Electronic Supporting Information

Physico-chemical and ion sensing properties of benzofurazan appended calix[4]arene in solution and on gold nanoparticles using spectroscopy, microscopy, and DFT computations in support of the species of recognition

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SI 01. Synthesis of the Precursors

Characterization data of P_1.

Yield: 86%, 10.1 g. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.72–7.75 (m, 4 H, PhtH), 7.56–7.60 (m, 4 H, PhtH), 7.44 (s, 2 H, OH), 7.02 (s, 4 H, ArH), 6.77 (s, 4 H, ArH), 4.30 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 4.09 (m, 8 H, CH_2N, OCH_2), 3.31 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 2.43 (quint, J = 7.2 Hz, 4 H, CH_2CH_2N), 1.27 (s, 18 H, ^{t}Bu), 0.93 (s, 18 H, ^{t}Bu) ppm.

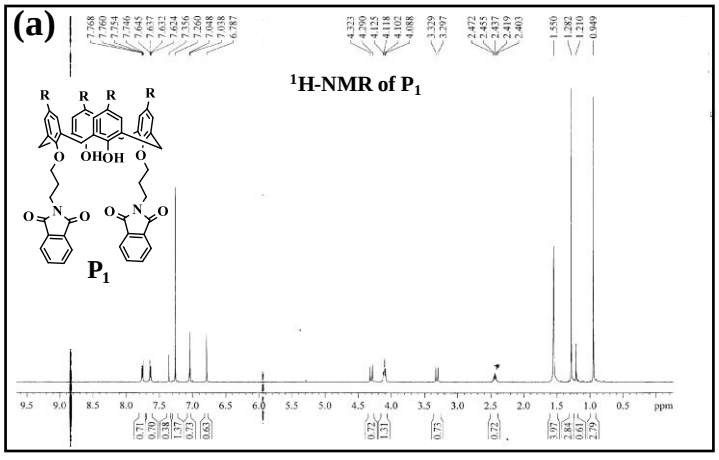
Characterization data of P_2: Yield: 78%. **^{1}H-NMR** (400MHz, $CDCl_3$): δ 1.23 (s, 18H, -$C(CH_3)_3$), 3.66 and 4.26 (bs, 8H, $ArCH_2Ar$), 7.14 and 7.59 (4s, 8H, ArH), 9.72 (s, 2H as , CHO), 10.28 (bs, 4H, D_2O exchs. OH). ESI-MS: LRMS peak for (m/z) for $C_{60}H_{58}N_2O_{10}$= 988.39 $[M]^+$ (calculated), 989.39 $[M+H]^+$ (obtained).

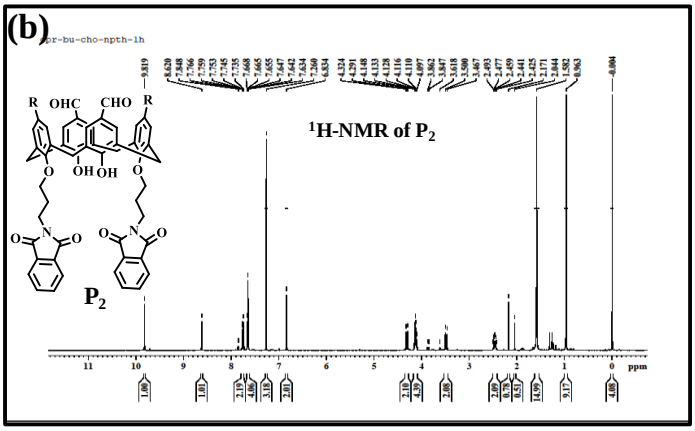
Characterization data of P_3. Yield: 75% ESI-MS: LRMS peak for (m/z) for $C_{60}H_{58}N_2O_{12}$ = 998.39 $[M]^+$ (calculated), 1021.38 $[M+Na]^+$ (obtained).**^{1}H-NMR** (400MHz, $CDCl_3$): δ 0.958 (s, 18H,$C(CH_3)_3$), 2.46 (quint., 4H,CH_2CH_2N), 3.47 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 4.14 (m, 8 H,CH_2N, OCH_2), 4.27 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 6.84 (s, 4 H,ArH), 7.25 (m, 4H, Phth), 7.63 (m, 4H, PhtH), 7.88 (s, 4 H, ArH) 8.48(s, 2 H, D_2O exchangable, OH)

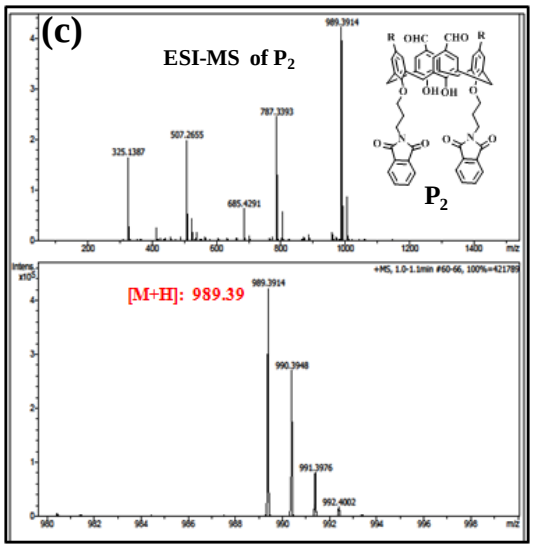
Characterization data of P_4. Yield: 70%. **^{1} H-NMR** (400 MHz, $CDCl_3$): δ 0.93 (s, 18H, −$C(CH_3)_3$), 1.9 (quint., 4H, $CH_2CH_2SCH_3$), 2.12 (s, 6H, SCH_3), 2.43 (quint., 4H, CH_2CH_2N), 2.6 (t, 4H, $NHCH_2CH_2$) 3.41 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 3.58 (m, 4H, $NHCH_2CH_2CH_2S$), 4.12 (m, 8 H, CH_2N, OCH_2), 4.28 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 6.5 (t, 2H, CONH), 6.85 (s, 4 H, ArH), 7.55 (s, 4 H, ArH), 7.65 (m, 4H, PhtH), 7.75 (m, 4H, PhtH), 8.15 (s, 2 H, D_2O exchangable, OH). ESI-MS: LRMS peak for (m/z) for $C_{68}H_{76}N_4O_{10}S_2$= 1172.50 $[M]^+$ (calculated), 1195.59 $[M+Na]^+$ (obtained).

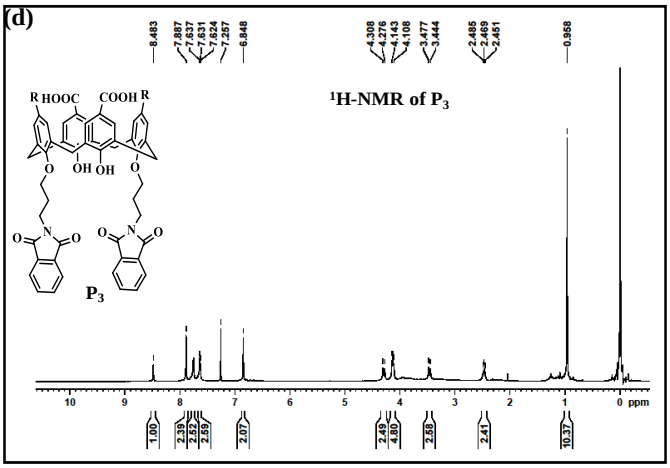
Characterization data of P_5. Yield: 90%. **^{1}H-NMR** (400 MHz, $CDCl_3$): δ 0.98 (s, 18H, $-C(CH_3)_3$), 1.9 (quint., 4H, $CH_2CH_2SCH_3$), 2.12 (m, 6H SCH_3, $CH_2CH_2CH_2N$), 2.61 (t, 4H, CH_2CH_2N), 3.16 (t, 4H, $NHCH_2CH_2$) 3.42 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 3.58 (m, 4H, $NHCH_2CH_2CH_2S$), 4.12 (t, 4 H, OCH_2), 4.28 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 6.48 (t, 2H, CONH), 6.85 (s, 4 H, ArH), 7.55 (s, 4 H, ArH). ESI-MS: LRMS calculated for $C_{52}H_{72}N_4O_6S_2$ $[M+H]^+$ 913.2852; found, 913.2815. ESI-MS: LRMS peak for (m/z) for $C_{50}H_{72}N_4O_6S_2$= 912.28 $[M]^+$ (calculated), 913.51 $[M+H]^+$ (obtained).

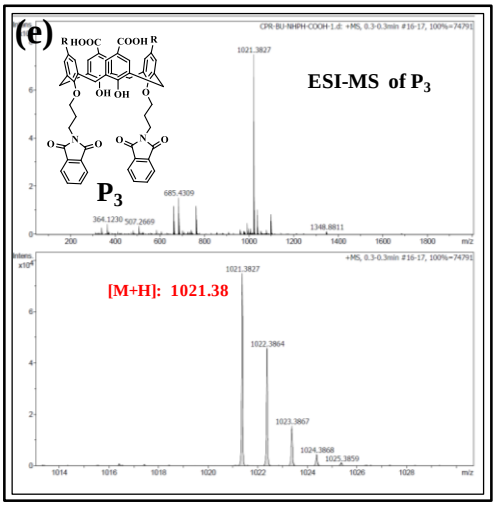
Characterization data for L. **^{1}H-NMR** (400 MHz, $CDCl_3$): δ 0.92 (s, 18H, $-C(CH_3)_3$), 1.9 (quint., 4H, $CH_2CH_2SCH_3$), 2.31 (m, 6H SCH_3, $CH_2CH_2CH_2N$), 2.61 (t, 4H, CH_2CH_2N), 3.83 (t, 4H, $NHCH_2CH_2$) 3.37 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 3.61 (m, 4H, $NHCH_2CH_2CH_2S$), 3.89 (t, 4 H, OCH_2), 4.11 (d, J = 13.0 Hz, 4 H, $ArCH_2Ar$), 4.78 (t, 2H, CONH), 6.21 (NBD-ArH), 6.48 (t, 2H, CONH), 6.79 (s, 4 H, ArH), 7.59 (s, 4 H, ArH), 8.29 (NBD-ArH).

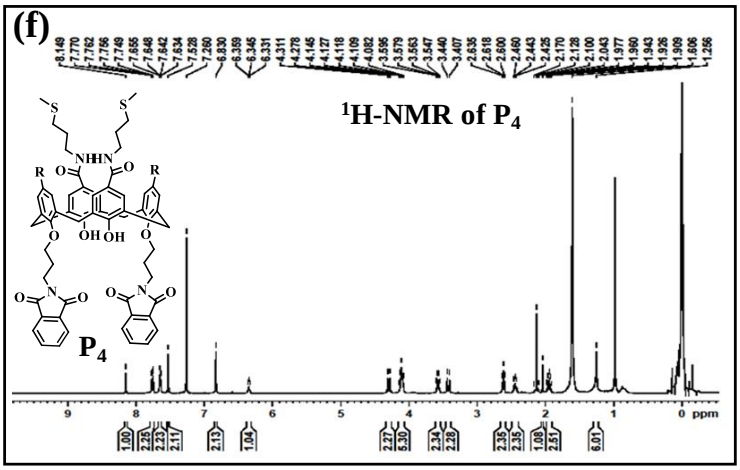


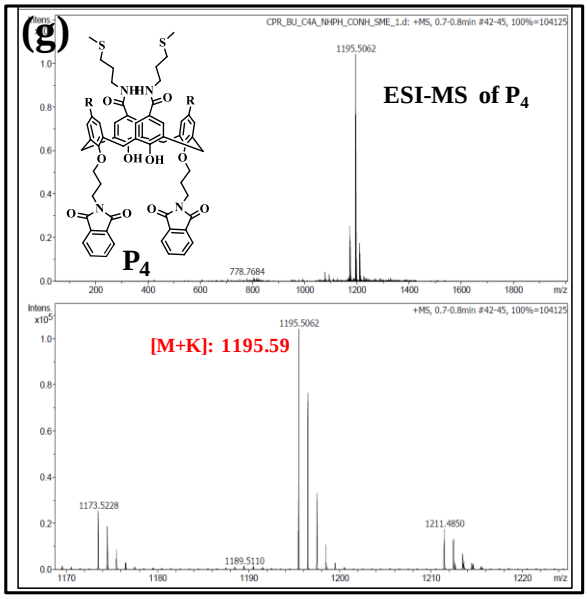

(b)
^{1}H-NMR of P$_2$
P$_2$

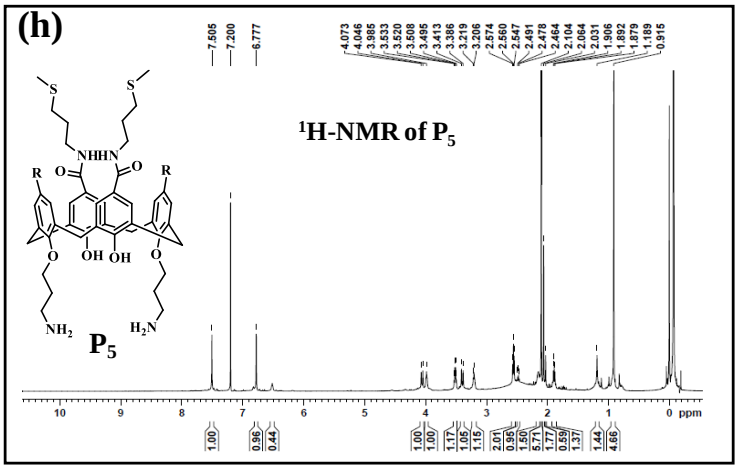

(c)
ESI-MS of P$_2$
989.3914
787.3393
507.2655
325.1387
685.4291
P$_2$
[M+H]: 989.39
990.3948
991.3976
992.4002

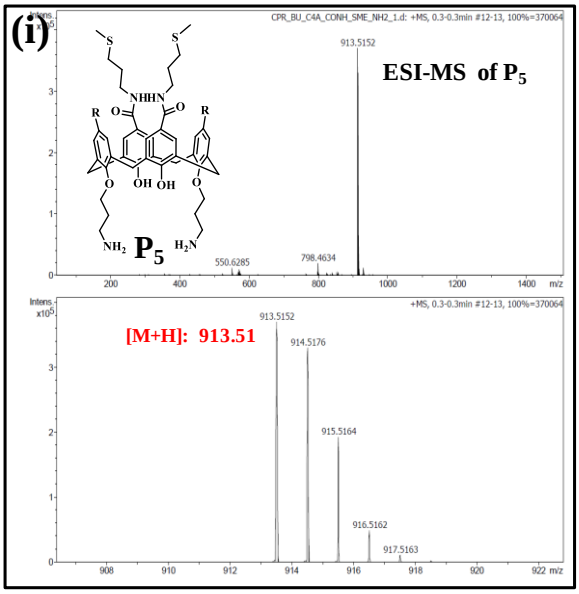

(d)
^{1}H-NMR of P$_3$
P$_3$

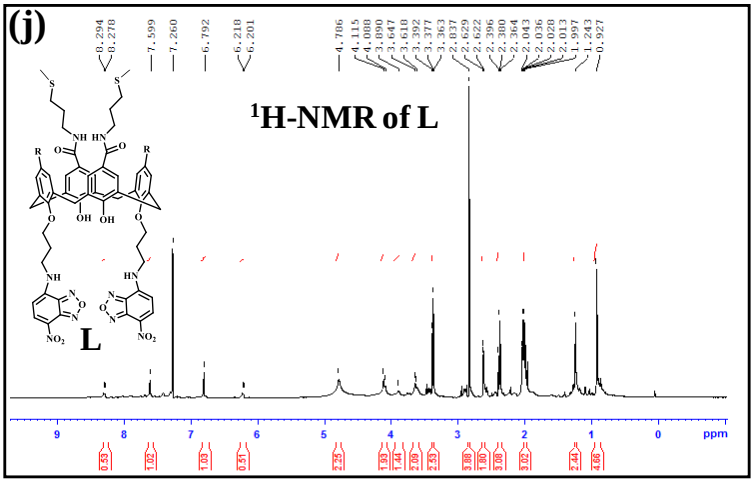

(e)
ESI-MS of P3
P3
[M+H]: 1021.38

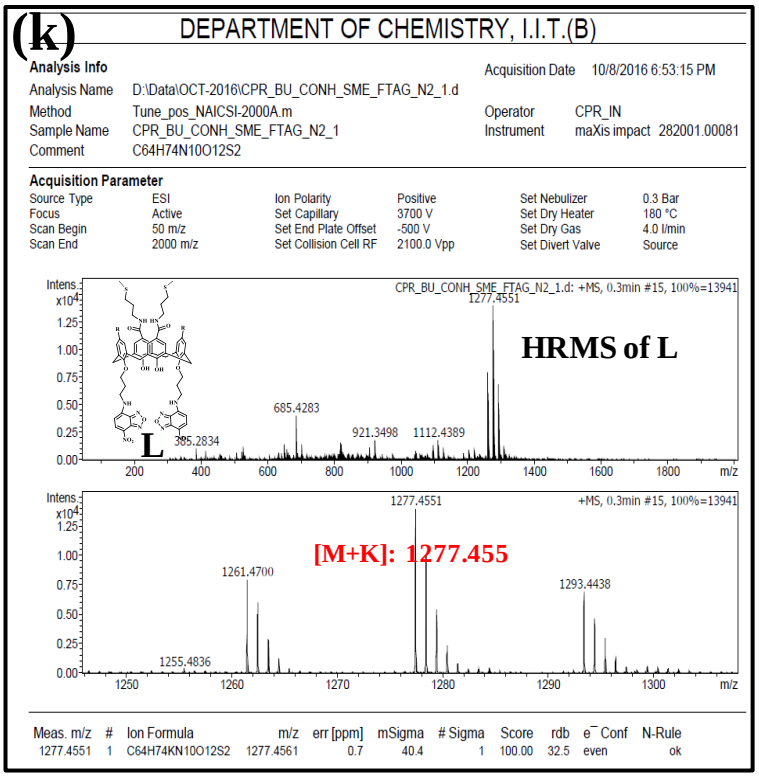

(f)
1H-NMR of P4
P4


(g)
ESI-MS of P4
P4
[M+K]: 1195.59
1195.5062
778.7684
1173.5228
1189.5110
1211.4850


(h)
1H-NMR of P5
P5
7.505
7.200
6.777
ppm


(i)
ESI-MS of P_5
P_5
913.5152
550.6285
798.4634
[M+H]: 913.51
914.5176
915.5164
916.5162
917.5163


(j)
^{1}H-NMR of L
L
8.294
8.278
7.599
7.260
6.792
6.218
6.201
4.786
4.115
4.088
3.890
3.647
3.618
3.392
3.377
3.363
3.337
2.629
2.622
2.396
2.380
2.364
2.043
2.036
2.028
2.013
1.997
1.243
0.927
ppm



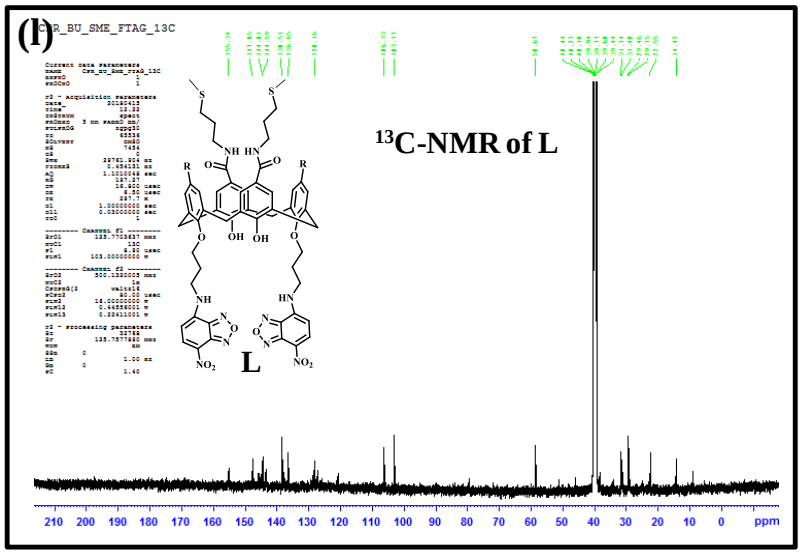


Figure S01. (a) ^{1}H NMR spectrum for P_1. (b) ^{1}H NMR spectrum for P_2. (c) ESI-MS spectrum for P_2. (d) ^{1}H NMR spectrum for P_3. (e) ESI-MS spectrum for P_3. (f) ^{1}H NMR spectrum for P_4. (g) ESI-MS spectrum for P_4. (h) ^{1}H NMR spectrum for P_5. (i) ESI-MS spectrum for P_5. (j) ^{1}H NMR spectrum for **L**. (k) HRMS spectrum for **L**. (l) ^{13}C NMR spectrum for **L**.

SI02. Plot of relative fluorescence intensity of L in different solvents.

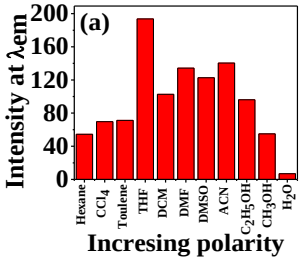


Figure S02. Histogram showing relative intensity of **L** in different solvents.

SI03. Fluorescence spectral traces for titration of L with different metal ions.

For all the titrations, the bulk concentration of both **L** and metal salt used were 6 x 10^{-4} M. For six different concentrations (1, 2, 4, 6, 8 and 10 equivalents) of metal ions fluorescence spectra were measured. In each titration 100 μL of of **L** (6 x 10^{-4} M) in ethanol was added with different volumes of metal ion solution being added and the final volume was made up to 3000 μL.

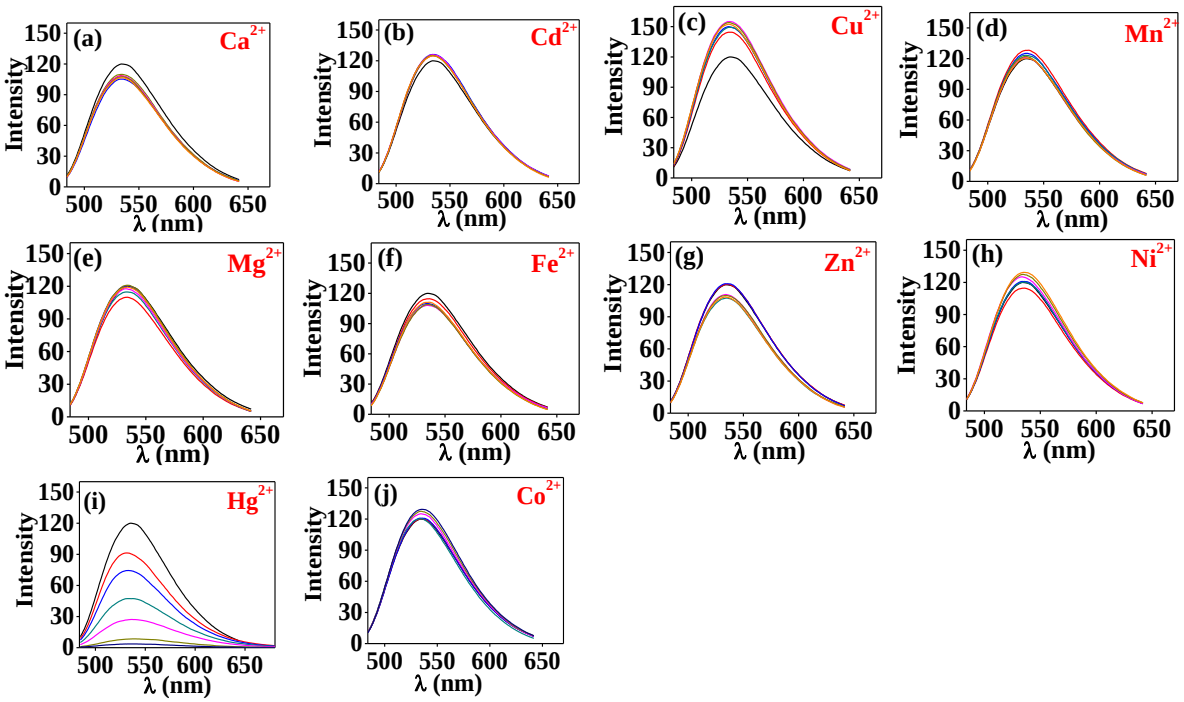


Figure S03. Fluorescence spectral traces for the titration of **L** with (a) Ca^{2+}, (b) Cd^{2+}, (c) Cu^{2+}, (d) Mn^{2+}, (e) Mg^{2+}, (f) Fe^{2+}, (g) Zn^{2+}, (h) Ni^{2+}, (i) Hg^{2+} and (j) Co^{2+}.

SI04. Plot of Fluorescence intensity with different ions and Job plot.

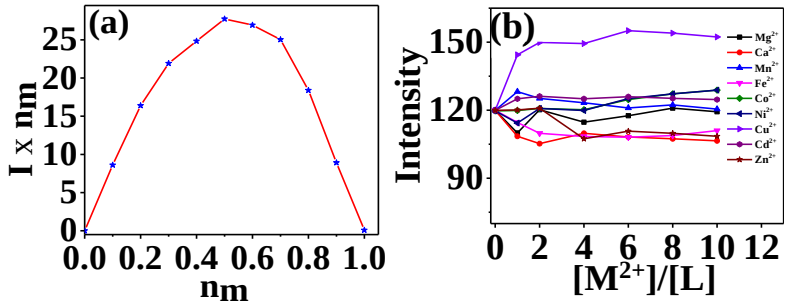


Figure S04. (a) Job plot of n_m *vs.* I x n_m where n_m is the mole fraction of the Hg^{2+} added and 'I' is the intensity. (b) Plot of $[M^{2+}]/L$ *vs.* fluorescence intensity at λ_{532} nm. Colour code for the plots: Mg^{2+} (black); Ca^{2+} (red); Mn^{2+} (blue); Fe^{2+} (cyan); Co^{2+} (orange); Ni^{2+} (dark-yellow); Cu^{2+} (magenta); Zn^{2+} (wine red); Cd^{2+} (navy blue); Hg^{2+} (green).

SI05. Competitive metal ion study & effect of counter anion of Hg^{2+}.

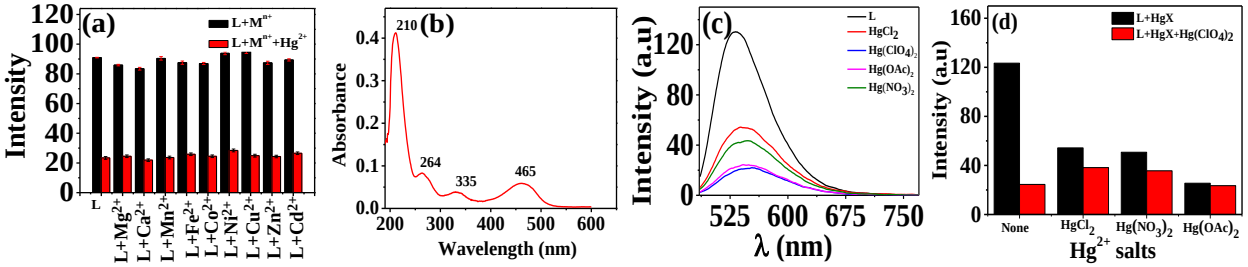


Figure S05. (a) Plot of fluorescence intensity where black bar indicates the **L** alone and in presence of different metal ions, i.e., {**L**+M^{n+}} and the red bar indicates the {**L**+M^{n+}}+Hg^{2+}; (b) Absorption spectrum of **L** in ethanol; (c) Fluorescence spectral traces for the titration of **L** with 10 equivalents of different counterions of Hg^{2+}; (d) Intensity plot of $Hg(ClO_4)_2$ salt in the presence of other salts possessing other anions, such as, chloride, nitrate and acetate.

SI06. Absorption spectral traces for the titration of L with different metal ions.

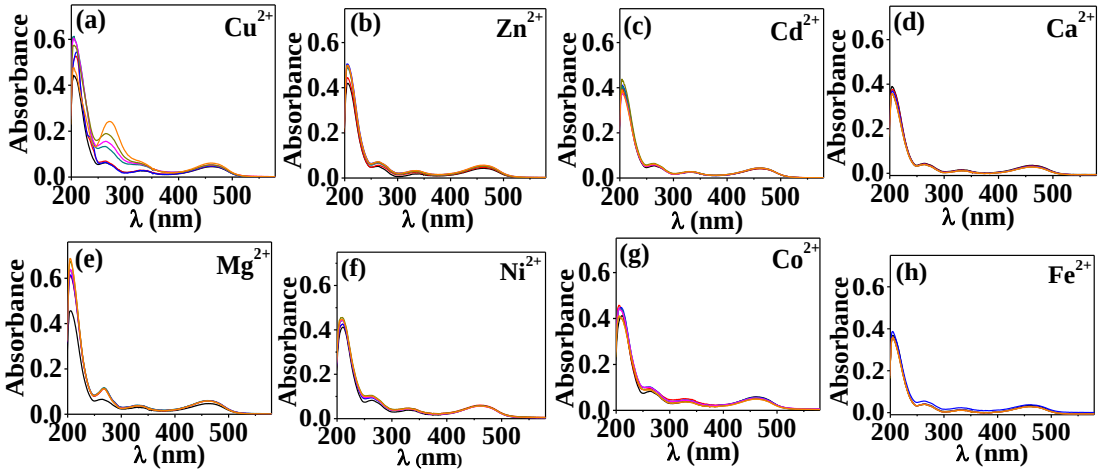


Figure S06. Absorption spectral traces for titration of **L** with (a) Cu^{2+}, (b) Zn^{2+}, (c) Cd^{2+}, (d) Ca^{2+}, (e) Mg^{2+}, (f) Ni^{2+}, (g) Co^{2+}, (h) Fe^{2+}.

SI07. SEM Micrographs of L and {L+Hg^{2+}} in ethanol.

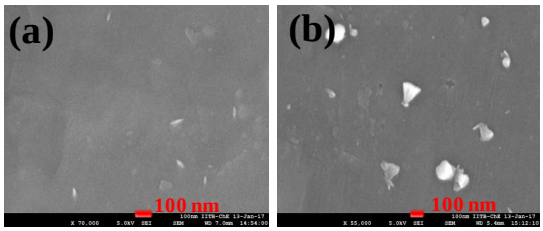


Figure S07. SEM micrographs of the samples taken from a thin layer on Al foil: (a) **L** taken in ethanol (the bar is 100 nm); (b) {**L**+Hg^{2+}} in ethanol (the bar is 100 nm).

SI08. EDAX analysis of $AuNP_{cit}$ and $AuNP_L$.

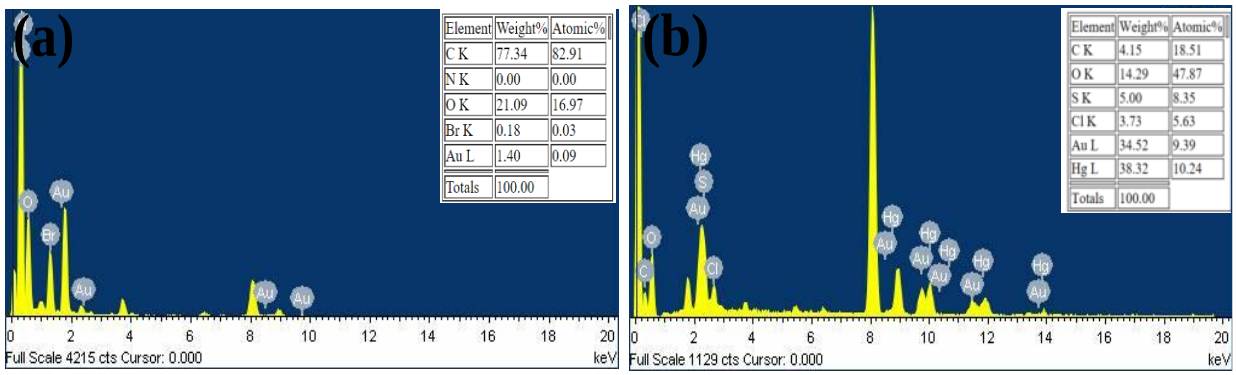


Figure S08. Elemental analysis of (a) $AuNP_{cit}$ and (b) $AuNP_L$

SI09. Absorption spectral traces for titration of $AuNP_L$ with metal ions.

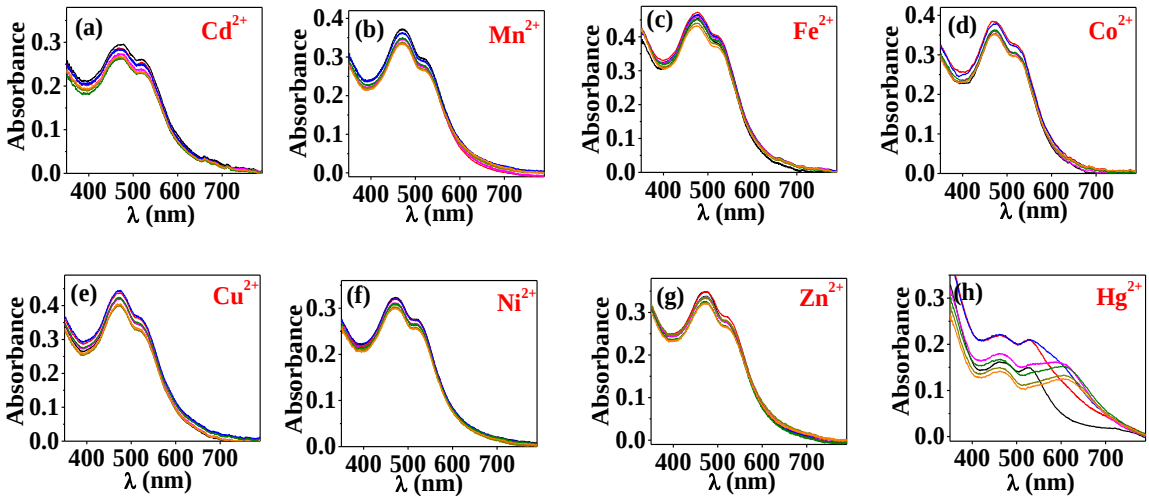


Figure S09. Absorption spectral traces for the titration of $AuNP_L$ with metal ions (a) Cd^{2+}; (b) Mn^{2+}; (c) Fe^{2+}; (d) Co^{2+}; (e) Cu^{2+}; (f) Ni^{2+}; (g) Zn^{2+}; (h) Hg^{2+}.

SI10. Fluorescence spectral traces for titration of AuNP$_L$ with metal ions.

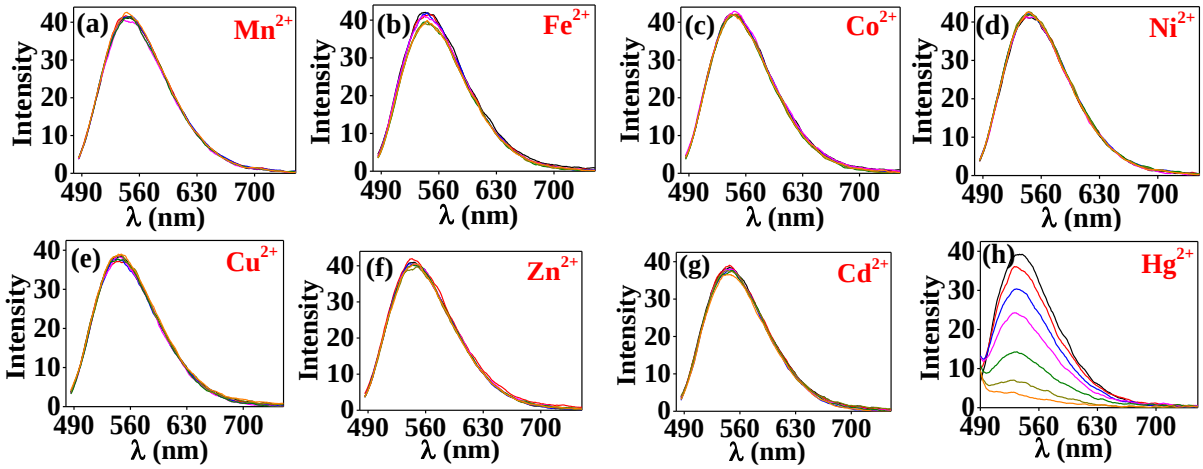


Figure S10. Fluorescence spectral traces for titration of AuNP$_L$ with different metal ions (a) Mn^{2+}; (b) Fe^{2+}; (c) Co^{2+}; (d) Ni^{2+}; (e) Cu^{2+}; (f) Zn^{2+}; (g) Cd^{2+}; (h) Hg^{2+}.

SI11. Limit of detection for Hg^{2+} on L and AuNP$_L$.

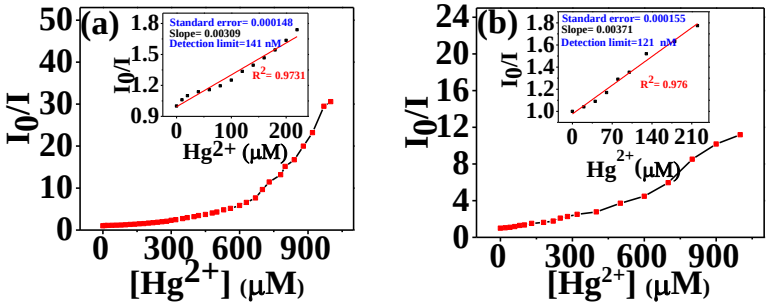


Figure S11. (a) Plot of I_0/I vs. concentration of Hg^{2+} (a) **L** (b) AuNP$_L$. Inset: Linear correlation betweeen I_0/I vs. concentration of Hg^{2+} for the calulation of detection limit in both the spectral profiles.

SI12. Fluorescence spectral traces for titration of $AuNP_L$ with different counter anions of Hg^{2+} salt.

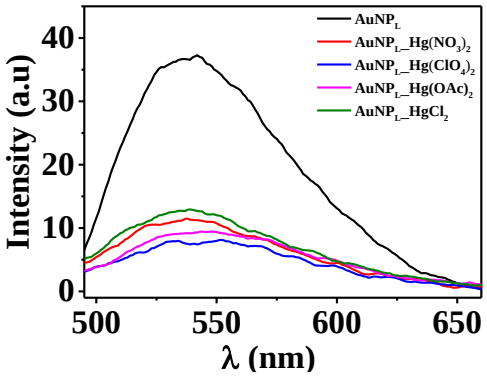


Figure S12. Fluorescence spectral traces for titration of $AuNP_L$ with different counter anions of Hg^{2+} ions.

SI13. DLS size distribution plot of L, $AuNP_L$ and $AuNP_{L+Hg2+}$.

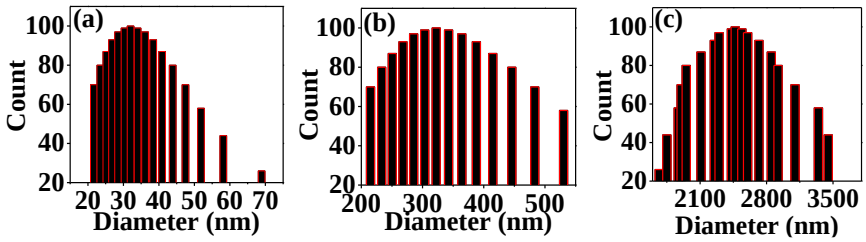


Figure S13. DLS distribution plot of (a) $AuNP_{cit}$ (b) $AuNP_L$ (c) $AuNP_{L+Hg2+}$.

SI14. Visible colour changes for reversibility studies of $L+Hg^{2+}$ complex.

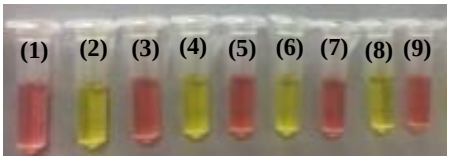


Figure S14. Photograph showing the colour changes depicting the reversibility of $L+Hg^{2+}$ complex. (1) $L+Hg^{2+}$; (2) 1 + TBAI; (3) 2 + Hg^{2+}; (4) 3 + TBAI; (5) 4 + Hg^{2+}; (6) 5 + TBAI; (7) 6 + Hg^{2+}; (8) 7 + TBAI; (9) 8+ Hg^{2+}.

SI15. Table S01. Fluorescence life time data fitted to three exponentials.

System	τ_1 (ns)	α_1	τ_2(ns)	α_2	τ_3 (ns)	α_3	$\chi 2$	τ (ns)
L	1.59	29.53	6.11	64.06	0.22	6.42	1.05	5.6±0.24
L+ Hg^{2+}	1.83	40.53	4.90	54.03	1.72	5.44	1.06	4.2±0.08
$AuNP_L$	1.27	43.86	3.98	46.31	0.15	9.83	1.14	3.3±0.11
$AuNP_{L+Hg2+}$	0.88	28.19	3.14	55.40	0.06	16.41	1.11	2.8±0.13

Note: τ_1, τ_2 and τ_3 are the three lifetimes with weightages of α1, α2 and α3, and τ is the average life time. The $\chi 2$ shows the correlation coefficient for the fitting.

SI16. Stereo view of {L+Hg^{2+}}.

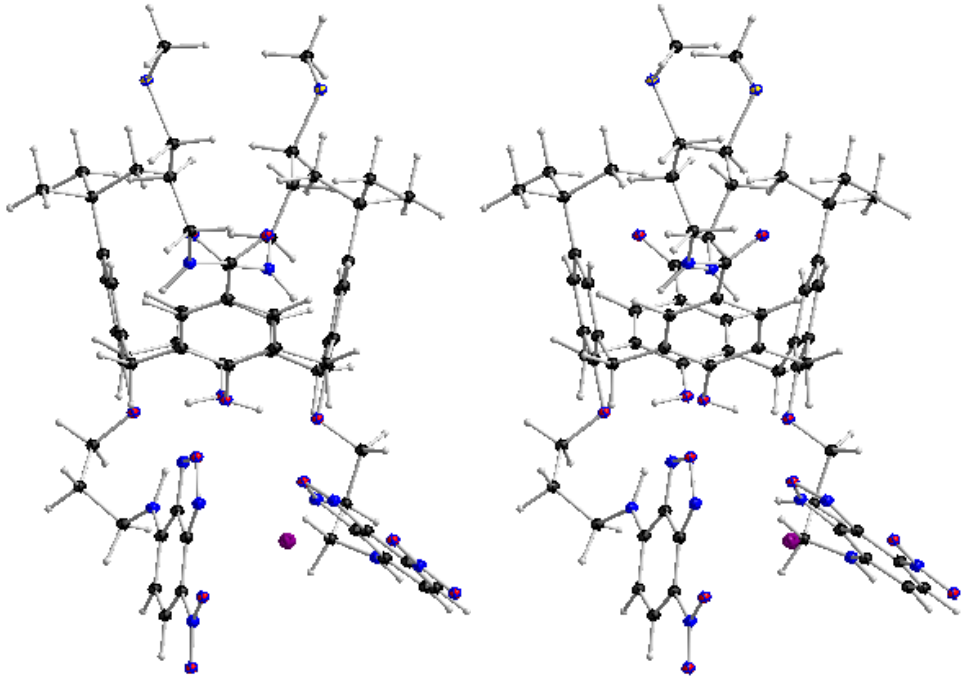


Figure S15. Stereoview of the {**L**+Hg^{2+}} complex.

SI17. DFT computational studies of L and its 1:1 complex with Hg^{2+}.

Table S02. Cartesian coordinates of the gas phase optimized structure of **L** at B3LYP/6-31G(d,p) level.

Atom		Coordinates (Å) of **L**		
		X	Y	Z
1	8	0.982633	-1.839863	-0.222818
2	1	0.392220	-1.651665	-0.972449
3	8	-0.008982	-1.344174	2.585913
4	8	-1.301880	0.330508	0.447053
5	1	-1.136941	-0.220093	1.231038
6	8	-1.025473	-0.815933	-2.379867
7	6	2.303457	-1.782952	-0.569735
8	6	2.735605	-1.600574	-1.898615
9	6	4.105043	-1.626332	-2.156897
10	1	4.472018	-1.493592	-3.169649
11	6	5.046104	-1.825796	-1.143122
12	6	4.589253	-1.945679	0.175017
13	1	5.297655	-2.026103	0.995921
14	6	3.229319	-1.913022	0.484109
15	6	2.759528	-1.949167	1.928844
16	1	3.591056	-2.294280	2.553192
17	1	1.950952	-2.672377	2.042218
18	6	0.937808	-0.319687	2.701996
19	6	2.287855	-0.589217	2.430105
20	6	3.208009	0.448250	2.589869
21	1	4.252236	0.235931	2.378281
22	6	1.472136	1.973212	3.200243
23	1	1.125058	2.963895	3.471156
24	6	2.834836	1.738193	2.995484
25	6	0.510776	0.965552	3.054959
26	6	3.909895	2.824864	3.182789
27	6	4.921457	2.362094	4.258249
28	1	5.697866	3.121466	4.402964
29	1	5.418594	1.429080	3.976336
30	1	4.423886	2.198724	5.219895
31	6	3.309674	4.169551	3.634849
32	1	2.605205	4.571366	2.899768
33	1	4.110149	4.905593	3.759477
34	1	2.790157	4.082905	4.594753
35	6	4.652381	3.053045	1.845188
36	1	3.959163	3.393807	1.069516
37	1	5.135997	2.141295	1.482917
38	1	5.428804	3.816533	1.965953
39	6	-0.967770	1.305837	3.206700
40	1	-1.118869	1.864247	4.135460
41	1	-1.563212	0.392513	3.296523

Atom		Coordinates (Å) of {**L**+Hg^{2+}}		
		X	Y	Z
1	8	-2.791698	-2.243544	1.326596
2	1	-2.409988	-1.859162	2.145316
3	8	-0.895964	-2.566726	-1.107310
4	8	-0.069341	-0.550728	0.780483
5	1	-0.172165	-1.235338	0.088522
6	8	-1.472327	-0.978731	3.431301
7	6	-4.129724	-2.171426	1.233736
8	6	-4.963294	-1.675891	2.272183
9	6	-6.337204	-1.693172	2.072923
10	1	-7.007673	-1.315388	2.838028
11	6	-6.912830	-2.206932	0.899721
12	6	-6.071211	-2.665420	-0.125512
13	1	-6.493532	-3.019744	-1.062031
14	6	-4.687786	-2.648682	0.013344
15	6	-3.769984	-3.087275	-1.109174
16	1	-4.350657	-3.666808	-1.834497
17	1	-2.994353	-3.740122	-0.706199
18	6	-1.741640	-1.657311	-1.753526
19	6	-3.124024	-1.891871	-1.802483
20	6	-3.924527	-0.958028	-2.468480
21	1	-4.995095	-1.137297	-2.496710
22	6	-2.032677	0.415393	-2.953739
23	1	-1.586772	1.313190	-3.366661
24	6	-3.406745	0.196822	-3.078047
25	6	-1.187364	-0.495309	-2.300669
26	6	-4.347976	1.169074	-3.812274
27	6	-5.094070	0.410265	-4.935936
28	1	-5.770291	1.090315	-5.463731
29	1	-5.696292	-0.415676	-4.545068
30	1	-4.392202	-0.002777	-5.667478
31	6	-3.586247	2.346666	-4.449227
32	1	-3.071240	2.957855	-3.700854
33	1	-4.291664	2.998802	-4.972385
34	1	-2.849034	2.006909	-5.184177
35	6	-5.376333	1.739866	-2.806142
36	1	-4.875892	2.293733	-2.004763
37	1	-5.979760	0.952539	-2.344002
38	1	-6.060722	2.426267	-3.315191
39	6	0.288824	-0.165892	-2.124580
40	1	0.703561	0.193964	-3.070128
41	1	0.852698	-1.063153	-1.853553

42	6	-1.598738	1.620577	0.754086
43	6	-1.487887	2.151544	2.055562
44	6	-1.830555	3.487181	2.258933
45	1	-1.749323	3.926468	3.248223
46	6	-2.284221	4.302592	1.218108
47	6	-2.355654	3.758126	-0.070959
48	1	-2.650120	4.378574	-0.913977
49	6	-2.014443	2.430507	-0.322386
50	6	-2.053790	1.857016	-1.726703
51	1	-2.578179	2.565901	-2.377773
52	1	-2.632397	0.932597	-1.724172
53	6	-0.183638	0.294217	-2.538229
54	6	-0.664138	1.588592	-2.289117
55	6	0.199632	2.662411	-2.515245
56	1	-0.179805	3.661373	-2.319568
57	6	1.518717	2.499899	-2.961079
58	6	1.974596	1.189644	-3.128901
59	1	3.002418	1.004068	-3.419690
60	6	1.149573	0.078746	-2.915103
61	6	2.402203	3.734053	-3.221513
62	6	1.745095	4.611142	-4.313797
63	1	2.355765	5.500130	-4.506438
64	1	0.748186	4.951464	-4.018199
65	1	1.645282	4.058200	-5.253652
66	6	3.815414	3.350288	-3.698555
67	1	3.790358	2.785444	-4.636159
68	1	4.351362	2.753172	-2.954023
69	1	4.402035	4.257148	-3.876241
70	6	2.538231	4.556827	-1.918908
71	1	3.160657	5.441769	-2.091785
72	1	3.006957	3.960554	-1.129546
73	1	1.568598	4.899536	-1.546490
74	6	1.746144	-1.323359	-3.019649
75	1	0.958703	-2.081168	-3.022100
76	1	2.273674	-1.425903	-3.972820
77	6	-0.291918	-1.986246	3.844474
78	1	-0.835704	-1.297004	4.503158
79	1	0.659982	-2.230602	4.336161
80	1	0.128184	-3.611530	0.869316
81	6	-1.109104	-3.247996	3.618458
82	1	-1.348146	-3.650599	4.610677
83	1	-2.061382	-2.996188	3.144411
84	1	-3.056017	-1.279773	-1.247842
85	6	-2.986603	-1.082988	-3.874719
86	1	-3.186599	-0.016271	-3.729309
87	1	-3.190065	-1.295444	-4.931412
88	6	-1.505769	-1.372365	-3.634448
89	1	-1.328491	-2.449554	-3.601110
90	1	-0.911743	-0.954705	-4.452316
91	6	-0.383099	-4.343224	2.812007
92	1	-0.758053	-5.329190	3.101394

42	6	0.232141	0.673441	0.299492
43	6	0.476910	0.919891	-1.079619
44	6	0.851138	2.202464	-1.457718
45	1	1.043995	2.433119	-2.500343
46	6	1.009281	3.234231	-0.520795
47	6	0.713991	2.980040	0.828294
48	1	0.774413	3.782400	1.558378
49	6	0.315020	1.720633	1.260544
50	6	-0.048058	1.477629	2.712818
51	1	0.354155	2.302867	3.309094
52	1	0.430385	0.568680	3.073940
53	6	-2.214176	0.206307	3.268905
54	6	-1.553659	1.396304	2.928801
55	6	-2.326149	2.549651	2.751629
56	1	-1.808648	3.467458	2.488769
57	6	-3.719873	2.568467	2.898696
58	6	-4.337683	1.348732	3.189491
59	1	-5.417274	1.295323	3.273735
60	6	-3.611918	0.162106	3.365879
61	6	-4.500908	3.882920	2.720672
62	6	-3.985781	4.925641	3.741765
63	1	-4.529787	5.868300	3.623783
64	1	-2.920930	5.140370	3.608559
65	1	-4.132487	4.577674	4.769230
66	6	-6.013507	3.695584	2.943350
67	1	-6.236813	3.334693	3.952730
68	1	-6.452905	2.998859	2.221824
69	1	-6.523372	4.655476	2.820645
70	6	-4.282196	4.416775	1.284481
71	1	-4.825721	5.356877	1.145217
72	1	-4.647074	3.701995	0.539262
73	1	-3.225819	4.610870	1.074388
74	6	-4.380398	-1.139022	3.568717
75	1	-3.757552	-1.905203	4.035480
76	1	-5.206293	-0.961781	4.262723
77	6	-0.525634	-3.700768	-1.928266
78	1	0.256660	-3.402513	-2.639328
79	1	-1.401352	-4.003863	-2.510460
80	1	2.235995	-6.079971	-1.986980
81	6	-0.067069	-4.849549	-1.034483
82	1	-0.716147	-4.880271	-0.152645
83	1	-0.225291	-5.794984	-1.568242
84	1	1.143321	-1.301024	2.801773
85	6	0.023965	-1.690626	5.274831
86	1	0.511159	-0.716137	5.384835
87	1	-0.058187	-2.110593	6.284928
88	6	-1.406348	-1.532003	4.773141
89	1	-1.887769	-2.517215	4.747613
90	1	-1.973229	-0.892829	5.455819
91	6	1.394462	-4.774927	-0.569934
92	1	1.549528	-5.475988	0.260301

93	1	0.684751	-4.338933	3.054848
94	6	-3.973257	-1.932223	-3.071584
95	1	-3.824930	-2.996060	-3.307061
96	1	-4.991140	-1.675250	-3.389395
97	7	-0.498049	-4.244162	1.362471
98	7	-3.883384	-1.728887	-1.626391
99	6	-4.798654	-2.248130	-0.775992
100	6	-4.666615	-2.044962	0.651555
101	6	-5.910792	-2.999646	-1.164849
102	6	-5.608594	-2.566645	1.610560
103	6	-6.835567	-3.507995	-0.226574
104	1	-6.067868	-3.237773	-2.208336
105	6	-6.729015	-3.314506	1.135169
106	1	-7.674868	-4.096283	-0.578879
107	6	-1.514767	-4.784998	0.660417
108	6	-1.452193	-4.781930	-0.786833
109	6	-2.651202	-5.398993	1.199182
110	6	-2.508291	-5.291890	-1.621691
111	6	-3.690265	-5.888092	0.381930
112	1	-2.781999	-5.454238	2.271934
113	6	-3.674505	-5.829758	-0.998571
114	1	-4.577109	-6.303148	0.847305
115	7	-3.714506	-1.401796	1.289558
116	7	-5.204131	-2.223445	2.822118
117	7	-0.459008	-4.374606	-1.546211
118	7	-2.135805	-5.171682	-2.885447
119	8	-0.871908	-4.615864	-2.820724
120	8	-4.042432	-1.507699	2.608301
121	7	-7.714568	-3.870967	2.031984
122	8	-8.682302	-4.459066	1.538530
123	8	-7.523767	-3.722552	3.241918
124	7	-4.829841	-6.226042	-1.758574
125	8	-5.776100	-6.745476	-1.156741
126	8	-4.815373	-5.993629	-2.972933
127	6	6.492334	-1.851741	-1.538318
128	8	6.881038	-1.349545	-2.590924
129	7	7.346054	-2.472198	-0.661106
130	1	6.950870	-3.006555	0.097005
131	6	-2.623796	5.724009	1.549665
132	8	-2.177716	6.277062	2.553214
133	7	-3.460430	6.364991	0.669811
134	1	-3.927402	5.815693	-0.034810
135	6	8.774939	-2.579148	-0.909092
136	6	9.614031	-1.881114	0.171208
137	1	8.946498	-2.123787	-1.887176
138	1	9.060130	-3.637696	-0.980301
139	6	11.112777	-1.992751	-0.117174
140	1	9.320609	-0.827070	0.223776
141	1	9.396399	-2.322799	1.152393
142	1	11.413066	-3.044711	-0.191242
143	1	11.353211	-1.505416	-1.068863

93	1	1.634466	-3.776344	-0.210103
94	6	0.926137	-2.629829	4.444008
95	1	0.330764	-3.436266	3.996224
96	1	1.650883	-3.098068	5.110384
97	7	2.325461	-5.129527	-1.647318
98	7	1.673481	-1.918536	3.409000
99	6	3.016655	-1.938996	3.262283
100	6	3.656837	-0.899230	2.483314
101	6	3.893373	-2.882582	3.817678
102	6	5.076430	-0.829757	2.274831
103	6	5.280819	-2.834249	3.588325
104	1	3.508203	-3.702782	4.409911
105	6	5.899922	-1.852143	2.831134
106	1	5.913945	-3.607700	4.009548
107	6	3.443825	-4.490792	-2.065554
108	6	3.763685	-3.123903	-1.706811
109	6	4.370580	-5.108685	-2.916286
110	6	4.953127	-2.459935	-2.185870
111	6	5.535035	-4.465943	-3.368241
112	1	4.194366	-6.133513	-3.227631
113	6	5.860147	-3.164566	-3.025605
114	1	6.227599	-5.003289	-4.006919
115	7	3.088394	0.140879	1.913944
116	7	5.334668	0.260981	1.567079
117	7	3.086596	-2.281286	-0.950983
118	7	4.957519	-1.224937	-1.703890
119	8	3.811452	-1.133730	-0.951303
120	8	4.104689	0.838836	1.352009
121	7	7.320043	-1.892117	2.615871
122	8	7.956380	-2.856511	3.029316
123	8	7.822137	-0.921953	2.011291
124	7	7.085938	-2.571113	-3.495160
125	8	7.832032	-3.243979	-4.197525
126	8	7.306278	-1.392826	-3.155307
127	6	-8.411403	-2.171433	0.808976
128	8	-9.057134	-1.356419	1.464955
129	7	-9.006619	-3.073357	-0.025447
130	1	-8.453364	-3.810812	-0.433463
131	6	1.433931	4.573817	-1.050268
132	8	1.193364	4.890489	-2.213391
133	7	2.090084	5.402110	-0.185758
134	1	2.383306	5.047425	0.711509
135	6	-10.460802	-3.136765	-0.140128
136	6	-11.014694	-2.127034	-1.159910
137	1	-10.882878	-2.931085	0.848415
138	1	-10.732307	-4.158740	-0.422033
139	6	-12.544944	-2.167901	-1.210571
140	1	-10.680204	-1.125507	-0.872605
141	1	-10.599528	-2.344185	-2.151063
142	1	-12.908252	-3.169878	-1.469941
143	1	-12.975249	-1.894858	-0.240152

144	6	-3.871327	7.747654	0.850343
145	6	-3.435980	8.644938	-0.317645
146	1	-3.414596	8.079222	1.785659
147	1	-4.961582	7.797962	0.976422
148	6	-3.874126	10.096822	-0.113164
149	1	-2.346412	8.593111	-0.418366
150	1	-3.861553	8.263776	-1.255083
151	1	-4.962562	10.156989	0.004498
152	1	-3.413521	10.509644	0.791526
153	6	-4.002286	12.746670	-1.007843
154	1	-3.763540	13.461235	-1.798385
155	1	-5.086240	12.728591	-0.865494
156	1	-3.514191	13.068278	-0.083876
157	6	13.769786	-1.457734	0.578069
158	1	14.459096	-1.017974	1.301904
159	1	13.995276	-2.523107	0.479752
160	1	13.907420	-0.960696	-0.385929
161	16	-3.377567	11.120529	-1.554627
162	16	12.081911	-1.193561	1.222290

144	6	2.582844	6.703753	-0.625567
145	6	1.519127	7.808589	-0.505375
146	1	2.895062	6.604856	-1.669669
147	1	3.464794	6.950950	-0.026464
148	6	2.045290	9.147244	-1.032430
149	1	0.636864	7.506279	-1.077962
150	1	1.214784	7.910151	0.542991
151	1	2.948799	9.459026	-0.494280
152	1	2.295551	9.076112	-2.097119
153	6	1.531440	11.817232	-1.763726
154	1	0.847506	12.664858	-1.696048
155	1	2.494946	12.095231	-1.327982
156	1	1.663849	11.543107	-2.813992
157	6	-14.959763	-1.067068	-2.147097
158	1	-15.439093	-0.395370	-2.861154
159	1	-15.333983	-2.083039	-2.299973
160	1	-15.188659	-0.736229	-1.130298
161	16	0.775266	10.449987	-0.833150
162	16	-13.170452	-0.986966	-2.461339
163	80	7.630913	-0.169527	-0.618220

Table S03. NBO atomic charges computed at B3LYP/6-31G(d,p)/SDD(Hg^{2+}) level.

No	Symbol	L	{L+Hg^{2+}}	L-{L+Hg^{2+}}
1	O	-0.722	-0.677	-0.04
2	H	0.526	0.528	0.00
3	O	-0.598	-0.605	0.01
4	O	-0.712	-0.690	-0.02
5	H	0.524	0.533	-0.01
6	O	-0.607	-0.609	0.00
7	C	0.371	0.408	-0.04
8	C	-0.083	-0.077	-0.01
9	C	-0.181	-0.175	-0.01
10	H	0.259	0.271	-0.01
11	C	-0.156	-0.101	-0.05
12	C	-0.215	-0.220	0.00
13	H	0.229	0.242	-0.01
14	C	-0.070	-0.042	-0.03
15	C	-0.475	-0.490	0.01
16	H	0.252	0.262	-0.01
17	H	0.244	0.265	-0.02
18	C	0.297	0.288	0.01
19	C	-0.049	-0.046	0.00
20	C	-0.213	-0.194	-0.02
21	H	0.233	0.239	-0.01
22	C	-0.216	-0.206	-0.01
23	H	0.244	0.250	-0.01

No	Symbol	L	{L+Hg^{2+}}	L-{L+Hg^{2+}}
83	H	0.259	0.253	0.01
84	H	0.454	0.451	0.00
85	C	-0.503	-0.506	0.00
86	H	0.248	0.257	-0.01
87	H	0.264	0.273	-0.01
88	C	-0.116	-0.112	0.00
89	H	0.233	0.218	0.01
90	H	0.231	0.244	-0.01
91	C	-0.276	-0.272	0.00
92	H	0.247	0.250	0.00
93	H	0.246	0.261	-0.01
94	C	-0.279	-0.269	-0.01
95	H	0.249	0.243	0.01
96	H	0.244	0.253	-0.01
97	N	-0.573	-0.569	0.00
98	N	-0.589	-0.568	-0.02
99	C	0.220	0.232	-0.01
100	C	0.094	0.091	0.00
101	C	-0.340	-0.313	-0.03
102	C	0.104	0.108	0.00
103	C	-0.149	-0.148	0.00
104	H	0.264	0.262	0.00
105	C	-0.006	0.017	-0.02

24	C	-0.016	-0.004	-0.01
25	C	-0.055	-0.050	-0.01
26	C	-0.065	-0.069	0.00
27	C	-0.672	-0.675	0.00
28	H	0.235	0.246	-0.01
29	H	0.231	0.229	0.00
30	H	0.237	0.242	-0.01
31	C	-0.688	-0.692	0.00
32	H	0.241	0.238	0.00
33	H	0.241	0.252	-0.01
34	H	0.236	0.240	0.00
35	C	-0.671	-0.673	0.00
36	H	0.236	0.236	0.00
37	H	0.234	0.231	0.00
38	H	0.234	0.245	-0.01
39	C	-0.495	-0.499	0.00
40	H	0.266	0.275	-0.01
41	H	0.253	0.258	0.00
42	C	0.376	0.415	-0.04
43	C	-0.089	-0.070	-0.02
44	C	-0.180	-0.180	0.00
45	H	0.258	0.271	-0.01
46	C	-0.160	-0.095	-0.07
47	C	-0.215	-0.216	0.00
48	H	0.228	0.242	-0.01
49	C	-0.071	-0.036	-0.03
50	C	-0.480	-0.477	0.00
51	H	0.250	0.264	-0.01
52	H	0.253	0.248	0.00
53	C	0.299	0.287	0.01
54	C	-0.046	-0.043	0.00
55	C	-0.211	-0.199	-0.01
56	H	0.234	0.238	0.00
57	C	-0.016	-0.002	-0.01
58	C	-0.216	-0.203	-0.01
59	H	0.244	0.250	-0.01
60	C	-0.065	-0.064	0.00
61	C	-0.065	-0.069	0.00
62	C	-0.672	-0.675	0.00
63	H	0.235	0.246	-0.01
64	H	0.232	0.229	0.00
65	H	0.237	0.243	-0.01
66	C	-0.688	-0.692	0.00
67	H	0.236	0.240	0.00
68	H	0.241	0.238	0.00
69	H	0.241	0.252	-0.01
70	C	-0.671	-0.673	0.00
71	H	0.234	0.245	-0.01
72	H	0.236	0.237	0.00
73	H	0.235	0.230	0.00
74	C	-0.497	-0.495	0.00

106	H	0.289	0.294	0.00
107	C	0.227	0.227	0.00
108	C	0.093	0.091	0.00
109	C	-0.339	-0.297	-0.04
110	C	0.106	0.116	-0.01
111	C	-0.151	-0.146	-0.01
112	H	0.258	0.264	-0.01
113	C	-0.007	0.012	-0.02
114	H	0.286	0.298	-0.01
115	N	-0.089	-0.070	-0.02
116	N	-0.062	-0.074	0.01
117	N	-0.079	-0.099	0.02
118	N	-0.074	-0.080	0.01
119	O	-0.150	-0.128	-0.02
120	O	-0.155	-0.117	-0.04
121	N	0.520	0.523	0.00
122	O	-0.410	-0.360	-0.05
123	O	-0.390	-0.428	0.04
124	N	0.520	0.527	-0.01
125	O	-0.411	-0.353	-0.06
126	O	-0.402	-0.421	0.02
127	C	0.692	0.681	0.01
128	O	-0.638	-0.611	-0.03
129	N	-0.661	-0.648	-0.01
130	H	0.415	0.425	-0.01
131	C	0.692	0.681	0.01
132	O	-0.640	-0.609	-0.03
133	N	-0.662	-0.646	-0.02
134	H	0.415	0.426	-0.01
135	C	-0.267	-0.268	0.00
136	C	-0.482	-0.487	0.01
137	H	0.264	0.258	0.01
138	H	0.225	0.243	-0.02
139	C	-0.599	-0.615	0.02
140	H	0.251	0.262	-0.01
141	H	0.234	0.244	-0.01
142	H	0.237	0.256	-0.02
143	H	0.242	0.260	-0.02
144	C	-0.266	-0.269	0.00
145	C	-0.482	-0.487	0.01
146	H	0.264	0.258	0.01
147	H	0.225	0.243	-0.02
148	C	-0.598	-0.616	0.02
149	H	0.250	0.261	-0.01
150	H	0.234	0.244	-0.01
151	H	0.237	0.256	-0.02
152	H	0.242	0.260	-0.02
153	C	-0.832	-0.847	0.01
154	H	0.257	0.277	-0.02
155	H	0.238	0.260	-0.02
156	H	0.239	0.260	-0.02

75	H	0.255	0.249	0.01
76	H	0.266	0.278	-0.01
77	C	-0.099	-0.103	0.00
78	H	0.222	0.219	0.00
79	H	0.212	0.233	-0.02
80	H	0.457	0.432	0.02
81	C	-0.507	-0.506	0.00
82	H	0.258	0.265	-0.01

157	C	-0.832	-0.847	0.01
158	H	0.258	0.276	-0.02
159	H	0.238	0.260	-0.02
160	H	0.239	0.260	-0.02
161	S	0.206	0.399	-0.19
162	S	0.206	0.399	-0.19
163	Hg	0.000	0.430	-1.57

+ve means gaining the charge and –ve means losing the charge on the atom

SI18. Two layer ONIOM computational data for 1:2 complex of Hg^{2+} and L.

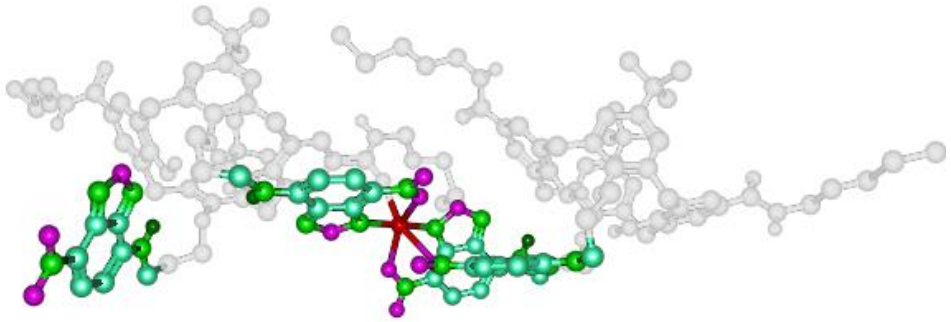


Figure S16. The optimized structure obtained from the two layered ONIOM partioning adopted for the 1:2 complex formation for the Hg^{2+} ion and **L**. The colour coded atoms are treated under B3LYP/6-31G(d,p)/SDD(Hg^{2+}) and the rest of the atoms (grey atoms) are treated under PM6 semi empirical method.

Table S04. Cartesian coordinates of the gas phase optimized structure {2**L**+Hg^{2+}} complex at B3LYP/6-31G(d,p)/SDD(Hg^{2+}) level.

Atom		Coordinates (Å) of {2**L**+Hg^{2+}}		
		X	Y	Z
1	8	6.530590	-1.129507	-0.344745
2	1	7.262589	-1.067243	0.358183
3	8	7.635273	-1.741018	-2.424668
4	8	9.775019	-1.153692	-0.302023
5	1	9.250384	-1.521234	-1.088367
6	8	8.561013	-1.297324	2.054414
7	6	5.516707	-0.240631	-0.148628
8	6	5.162264	0.241129	1.135314
9	6	3.966358	0.948901	1.269265
10	1	3.652441	1.306787	2.253178
11	6	3.148445	1.170707	0.152908
12	6	3.563188	0.790157	-1.130203
13	1	2.947340	1.039980	-1.998290
14	6	4.753938	0.083047	-1.301807
15	6	5.200701	-0.323145	-2.678534
16	1	4.435700	-0.051372	-3.438223
17	1	5.298980	-1.428459	-2.728245
18	6	7.710425	-0.448911	-2.970901
19	6	6.520627	0.296874	-3.053494

Atom		Coordinates (Å) of {2**L**+Hg^{2+}}		
		X	Y	Z
164	1	-9.551198	-0.766556	1.514763
165	8	-8.348273	-2.664756	-1.864675
166	8	-7.327539	-0.161185	0.158949
167	1	-7.846988	-0.756857	-0.456691
168	8	-8.367584	0.345031	3.009990
169	6	-11.332592	-0.863062	0.625037
170	6	-11.998728	0.016571	1.504841
171	6	-13.334684	0.338365	1.234230
172	1	-13.874922	1.030724	1.886089
173	6	-13.987334	-0.206273	0.124721
174	6	-13.307643	-1.054826	-0.757409
175	1	-13.820539	-1.444575	-1.638775
176	6	-11.968386	-1.378764	-0.531691
177	6	-11.190219	-2.182722	-1.538655
178	1	-11.868523	-2.738865	-2.218558
179	1	-10.582882	-2.949629	-1.005920
180	6	-8.904420	-1.477482	-2.379145
181	6	-10.293187	-1.263079	-2.326507
182	6	-10.802917	-0.121016	-2.952117

20	6	6.589133	1.624403	-3.485379
21	1	5.673914	2.213930	-3.530857
22	6	8.982778	1.439993	-3.752673
23	1	9.950805	1.885808	-4.000343
24	6	7.813929	2.206816	-3.851438
25	6	8.953119	0.110011	-3.311265
26	6	7.861633	3.675774	-4.288624
27	6	6.641442	4.010654	-5.169965
28	1	6.715673	5.029795	-5.567776
29	1	5.694719	3.946436	-4.614655
30	1	6.576061	3.333797	-6.029304
31	6	9.132697	3.988600	-5.095529
32	1	10.046096	3.851529	-4.502422
33	1	9.142212	5.031553	-5.435071
34	1	9.214911	3.359212	-5.988198
35	6	7.840435	4.533809	-3.008610
36	1	8.711783	4.321850	-2.375610
37	1	6.946037	4.351639	-2.407324
38	1	7.872880	5.602496	-3.248385
39	6	10.239358	-0.658957	-3.159310
40	1	10.799388	-0.656393	-4.121329
41	1	10.049917	-1.737255	-2.948406
42	6	10.761010	-0.288815	-0.702506
43	6	11.065345	-0.051039	-2.060611
44	6	12.114840	0.821197	-2.365946
45	1	12.370909	1.029525	-3.408253
46	6	12.834369	1.448288	-1.343049
47	6	12.506959	1.226882	-0.000344
48	1	13.058307	1.747172	0.784818
49	6	11.463664	0.361820	0.339134
50	6	11.060250	0.165295	1.772900
51	1	11.835872	0.562570	2.462122
52	1	10.990786	-0.929563	1.991894
53	6	8.544967	0.103344	2.172093
54	6	9.738247	0.834362	2.037837
55	6	9.667922	2.231825	2.094986
56	1	10.588896	2.809725	1.980317
57	6	8.448225	2.902599	2.273821
58	6	7.269885	2.146762	2.355042
59	1	6.305423	2.645933	2.448062
60	6	7.301258	0.748568	2.299546
61	6	8.428512	4.435457	2.310578
62	6	9.605153	4.957685	3.155638
63	1	9.572211	6.049878	3.250009
64	1	10.576651	4.713308	2.711695
65	1	9.589211	4.543627	4.169468
66	6	7.122584	4.976503	2.922729
67	1	6.975230	4.607311	3.943413
68	1	6.245168	4.707215	2.328201
69	1	7.145411	6.072029	2.979594
70	6	8.559467	4.931328	0.857891

183	1	-11.882991	0.048129	-2.946110
184	6	-8.571886	0.646836	-3.471209
185	1	-7.890517	1.403605	-3.859923
186	6	-9.959432	0.823871	-3.563125
187	6	-8.027234	-0.494408	-2.869282
188	6	-10.594059	2.017506	-4.287652
189	6	-11.476307	1.471997	-5.427278
190	1	-11.918085	2.288698	-6.011202
191	1	-12.309324	0.867519	-5.053528
192	1	-10.901543	0.850458	-6.121713
193	6	-9.540698	2.963916	-4.892012
194	1	-8.884998	3.390278	-4.126680
195	1	-10.025563	3.807425	-5.400563
196	1	-8.921254	2.459979	-5.640892
197	6	-11.450916	2.810012	-3.284774
198	1	-10.837410	3.226011	-2.467534
199	1	-12.234287	2.197263	-2.825226
200	1	-11.956891	3.651101	-3.773428
201	6	-6.540793	-0.633791	-2.673844
202	1	-6.035921	-0.636535	-3.664448
203	1	-6.300610	-1.627827	-2.229059
204	6	-6.456391	0.669919	-0.475987
205	6	-5.992265	0.460564	-1.796535
206	6	-4.981663	1.299277	-2.280151
207	1	-4.584336	1.126071	-3.281260
208	6	-4.463523	2.328462	-1.486117
209	6	-4.984268	2.559772	-0.199949
210	1	-4.581865	3.386160	0.394676
211	6	-5.984685	1.744671	0.323052
212	6	-6.516889	1.982946	1.711235
213	1	-5.945199	2.800043	2.205010
214	1	-6.342049	1.053965	2.314089
215	6	-8.912353	1.467004	2.362528
216	6	-7.984848	2.316554	1.724524
217	6	-8.464704	3.449315	1.064138
218	1	-7.753961	4.119775	0.577516
219	6	-9.841424	3.731339	0.999905
220	6	-10.739727	2.816503	1.560764
221	1	-11.817493	2.975897	1.470285
222	6	-10.295141	1.661669	2.223670
223	6	-10.305219	5.025468	0.320100
224	6	-9.832092	6.207938	1.188470
225	1	-10.153994	7.164589	0.759620
226	1	-8.742863	6.245226	1.279039
227	1	-10.248543	6.153305	2.200218
228	6	-11.834090	5.094353	0.172694
229	1	-12.345095	5.093147	1.141732
230	1	-12.230845	4.261199	-0.419235
231	1	-12.139734	6.016464	-0.337768
232	6	-9.676598	5.112732	-1.083922
233	1	-10.005976	6.018130	-1.606716

71	1	8.553241	6.026148	0.810759
72	1	7.740974	4.566390	0.229855
73	1	9.497341	4.597061	0.398098
74	6	6.017219	-0.037578	2.339534
75	1	6.219513	-1.131169	2.399608
76	1	5.470368	0.201515	3.278828
77	6	7.716481	-2.811809	-3.417052
78	1	8.782705	-2.907350	-3.711858
79	1	7.110617	-2.551564	-4.298888
80	1	5.619349	-3.159994	-0.916667
81	6	7.228637	-4.053111	-2.671412
82	1	7.766858	-4.944942	-3.077270
83	1	7.574151	-3.986699	-1.612330
84	1	10.064922	-2.961925	1.171238
85	6	9.940544	-2.464064	3.685427
86	1	10.664676	-1.687432	3.326805
87	1	10.061947	-2.475196	4.790704
88	6	8.525677	-2.017115	3.323638
89	1	7.853562	-2.864567	3.097205
90	1	8.082452	-1.385573	4.112280
91	6	5.731550	-4.286782	-2.758523
92	1	5.493668	-5.360407	-2.731519
93	1	5.315915	-3.864263	-3.685619
94	6	10.328417	-3.830088	3.133562
95	1	9.616293	-4.603825	3.474028
96	1	11.327155	-4.114638	3.505373
97	7	5.044055	-3.645791	-1.606827
98	7	10.349849	-3.808510	1.665075
99	6	10.646215	-4.907295	0.939238
100	6	10.557331	-4.866823	-0.504877
101	6	11.034412	-6.141066	1.473189
102	6	10.824085	-6.009419	-1.343850
103	6	11.307691	-7.255579	0.651576
104	1	11.130085	-6.264405	2.543703
105	6	11.213605	-7.234917	-0.725310
106	1	11.603908	-8.192778	1.109227
107	6	3.719949	-3.490562	-1.536532
108	6	3.113927	-2.892071	-0.358442
109	6	2.805079	-3.877032	-2.536954
110	6	1.709544	-2.568027	-0.272592
111	6	1.449216	-3.560595	-2.441577
112	1	3.151999	-4.388152	-3.421616
113	6	0.868817	-2.885136	-1.366078
114	1	0.790589	-3.827647	-3.259010
115	7	10.201496	-3.851905	-1.255985
116	7	10.621841	-5.656346	-2.602594
117	7	3.709914	-2.580713	0.768728
118	7	1.531511	-2.060522	0.940223
119	8	2.767084	-2.059934	1.573094
120	8	10.242654	-4.331026	-2.534184
121	7	11.476706	-8.431740	-1.494219
234	1	-9.975099	4.250309	-1.705439
235	1	-8.584089	5.139155	-1.051990
236	6	-11.309758	0.647281	2.684486
237	1	-10.849558	-0.143614	3.318947
238	1	-12.055305	1.141295	3.348902
239	6	-8.494828	-3.768634	-2.819928
240	1	-8.206362	-3.412627	-3.826287
241	1	-9.557909	-4.066935	-2.823756
242	1	-8.116647	-3.764115	0.389809
243	6	-7.567536	-4.874039	-2.327473
244	1	-7.585831	-5.706751	-3.067344
245	1	-6.518035	-4.506078	-2.331940
246	1	-5.954451	1.063164	3.902015
247	6	-8.043777	1.281183	5.282131
248	1	-7.954224	2.218020	4.683268
249	1	-8.753960	1.558206	6.095671
250	6	-8.664370	0.182608	4.418672
251	1	-8.227175	-0.819419	4.598946
252	1	-9.763291	0.130100	4.555261
253	6	-7.947380	-5.414500	-0.950266
254	1	-7.515164	-6.408190	-0.776756
255	1	-9.034757	-5.499022	-0.840093
256	6	-6.715133	0.892975	5.910235
257	1	-6.766394	-0.107416	6.367748
258	1	-6.420836	1.614844	6.686437
259	7	-7.488562	-4.520158	0.127683
260	7	-5.666921	0.881858	4.867070
261	6	-4.404870	0.498071	5.068651
262	6	-3.465265	0.554257	3.968298
263	6	-3.873996	0.022210	6.283867
264	6	-2.119233	0.064411	4.060122
265	6	-2.562106	-0.451366	6.361224
266	1	-4.493454	-0.023072	7.166817
267	6	-1.665774	-0.468844	5.289361
268	1	-2.201615	-0.847987	7.302779
269	6	-6.208822	-4.383022	0.502134
270	6	-5.865197	-3.388196	1.496079
271	6	-5.129047	-5.148325	0.021829
272	6	-4.517112	-3.124009	1.913914
273	6	-3.815042	-4.894322	0.428622
274	1	-5.299070	-5.925385	-0.709006
275	6	-3.460444	-3.900620	1.338388
276	1	-3.011692	-5.480006	-0.001804
277	7	-3.684399	1.023440	2.761998
278	7	-1.578983	0.257392	2.863660
279	7	-6.685677	-2.596993	2.149420
280	7	-4.548121	-2.162994	2.818271
281	8	-5.891016	-1.849004	2.948199
282	8	-2.554196	0.844846	2.065153
283	7	-0.355310	-1.004891	5.444859
284	8	-0.015796	-1.428996	6.544368

122	8	11.821527	-9.444690	-0.881163
123	8	11.329425	-8.353075	-2.714624
124	7	-0.515003	-2.535056	-1.401293
125	8	-1.197129	-2.937288	-2.342091
126	8	-0.974802	-1.821918	-0.487865
127	6	1.774143	1.710299	0.366489
128	8	0.909726	0.987585	0.916272
129	7	1.493965	2.988157	-0.030276
130	1	2.199262	3.551979	-0.512993
131	6	13.896665	2.438246	-1.721461
132	8	13.671806	3.423535	-2.405759
133	7	15.173491	2.135725	-1.259748
134	1	15.355496	1.313686	-0.695762
135	6	0.143039	3.586025	0.154146
136	6	-0.201775	3.753704	1.645097
137	1	-0.624019	2.930138	-0.340354
138	1	0.107779	4.562156	-0.377968
139	6	-1.676579	4.089591	1.807202
140	1	0.048840	2.811381	2.186020
141	1	0.433637	4.535906	2.103565
142	1	-1.856292	5.179760	1.793998
143	1	-2.289813	3.672469	0.965962
144	6	16.311617	3.059194	-1.486714
145	6	16.757838	3.702088	-0.160971
146	1	16.003313	3.847287	-2.217937
147	1	17.146685	2.491190	-1.953637
148	6	17.940327	4.632470	-0.390433
149	1	15.906639	4.260860	0.284302
150	1	17.021642	2.914485	0.574994
151	1	18.804670	4.100200	-0.827159
152	1	17.682750	5.458945	-1.078323
153	6	19.805932	6.336864	0.879821
154	1	20.142714	6.790806	1.823182
155	1	20.640617	5.759673	0.467860
156	1	19.557441	7.147168	0.186205
157	6	-1.717954	4.390130	4.652461
158	1	-2.084733	3.992831	5.607893
159	1	-0.622760	4.395000	4.680429
160	1	-2.069938	5.424853	4.558914
161	16	18.377923	5.297498	1.250994
162	16	-2.352902	3.346241	3.321410
163	8	-10.047058	-1.301427	0.822569

285	8	0.407752	-1.008680	4.449235
286	7	-2.098947	-3.641375	1.610737
287	8	-1.219808	-4.320271	1.069557
288	8	-1.842972	-2.699088	2.406791
289	6	-15.398476	0.221526	-0.158024
290	8	-15.715609	1.387338	-0.326764
291	7	-16.331453	-0.809965	-0.182307
292	1	-16.061354	-1.776612	-0.043594
293	6	-3.314953	3.180970	-1.902475
294	8	-2.498961	3.619907	-1.089945
295	7	-3.177255	3.487283	-3.250958
296	1	-3.822035	3.143145	-3.952367
297	6	-17.749794	-0.553585	-0.533572
298	6	-18.093297	-1.190770	-1.892012
299	1	-17.925436	0.550638	-0.564544
300	1	-18.398143	-0.963022	0.272634
301	6	-19.550858	-0.935215	-2.248228
302	1	-17.425807	-0.773949	-2.676807
303	1	-17.886220	-2.280692	-1.865095
304	1	-20.239336	-1.333835	-1.481294
305	1	-19.763300	0.145240	-2.349247
306	6	-2.060846	4.348761	-3.715088
307	6	-0.706747	3.617550	-3.609120
308	1	-2.037960	5.274180	-3.089159
309	1	-2.262347	4.661485	-4.762162
310	6	0.435164	4.563526	-3.946229
311	1	-0.600609	3.218808	-2.574655
312	1	-0.696818	2.733010	-4.276988
313	1	0.453558	4.810199	-5.024664
314	1	0.355442	5.520806	-3.396927
315	6	3.241641	4.797106	-4.186430
316	1	4.226161	4.294369	-4.117053
317	1	3.056102	4.998919	-5.248717
318	1	3.311541	5.754723	-3.658238
319	6	-21.560243	-1.398987	-4.183983
320	1	-21.824169	-1.875997	-5.139215
321	1	-22.231887	-1.794009	-3.414338
322	1	-21.732157	-0.322186	-4.287250
323	16	1.983893	3.719338	-3.470972
324	16	-19.830550	-1.781614	-3.839914
325	80	-0.054133	-0.906692	1.866436