Supporting Information

Synthesis of Triazole Linked Fluorescent Amino Acid and Carbohydrate Bio-Conjugates: A Highly Sensitive and Skeleton Selective Multi-Responsive Chemosensor for Cu(II) and Pb(II)/Hg(II) Ion

Arunabha Thakur, Pranab Deb, Dipendu Mandal, Bijan Mondal and Sundargopal Ghosh*

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600 036, India.

Phone: (+91) 44 2257 4230; Fax: (+91) 44 2257 4202

Email: sghosh@iitm.ac.in

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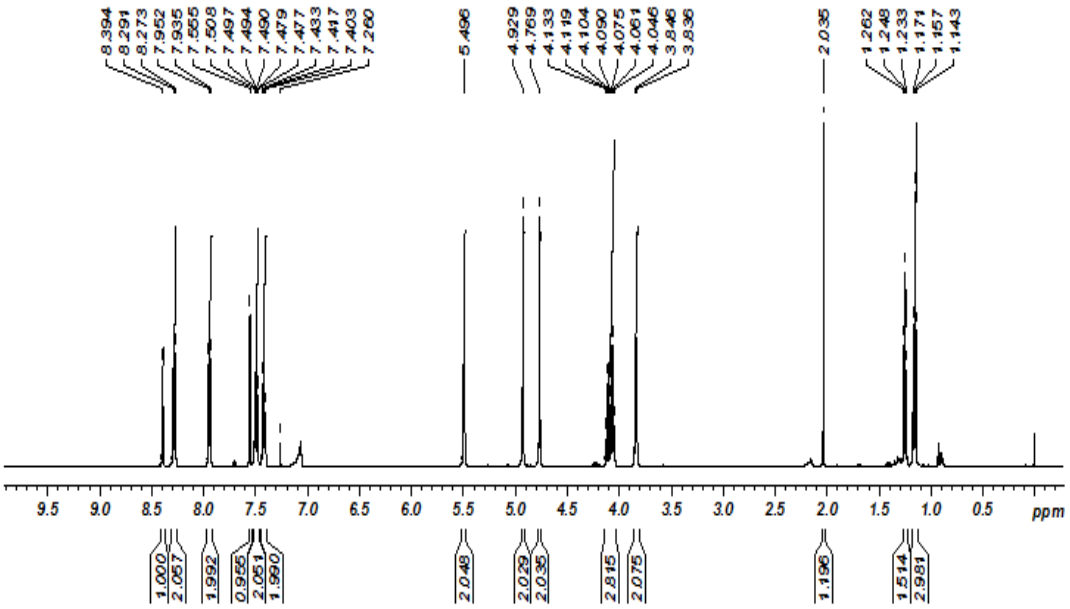
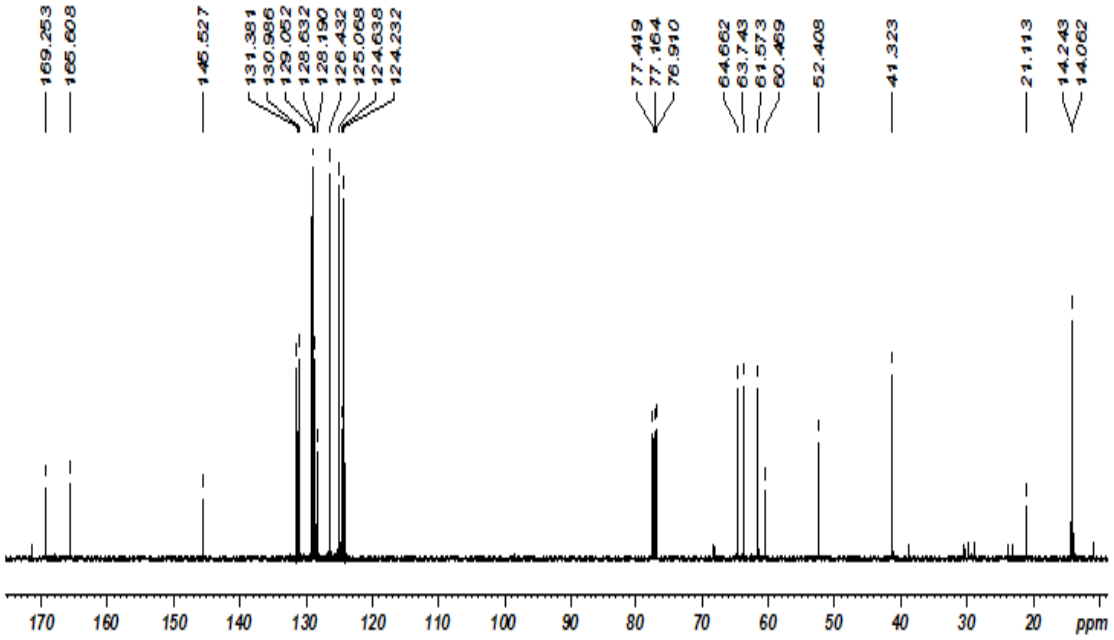
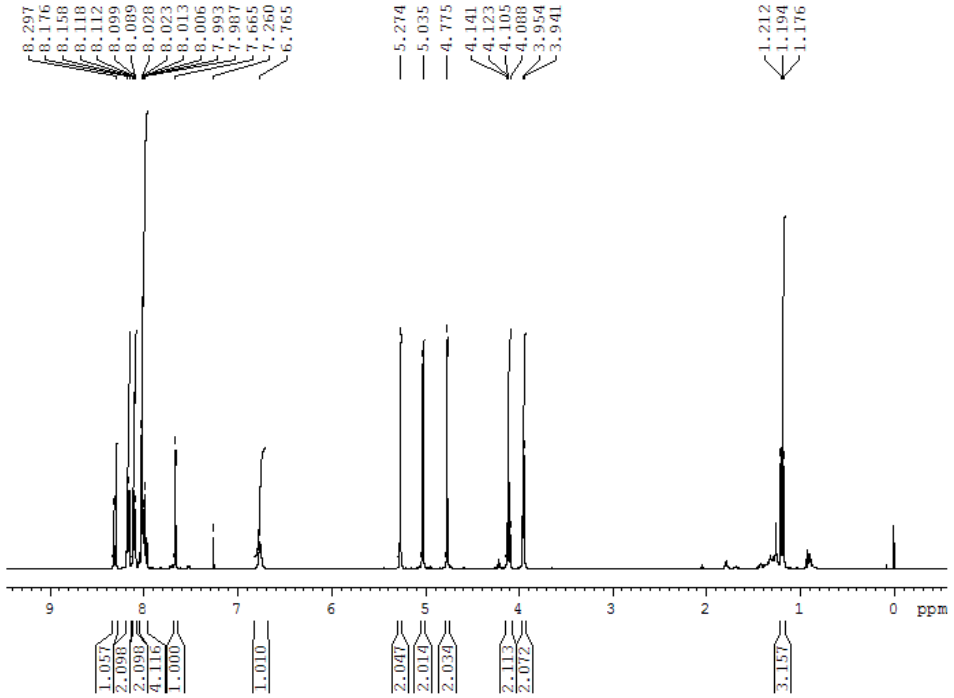
^{1}H NMR spectra of 3 (C*D*Cl$_3$)



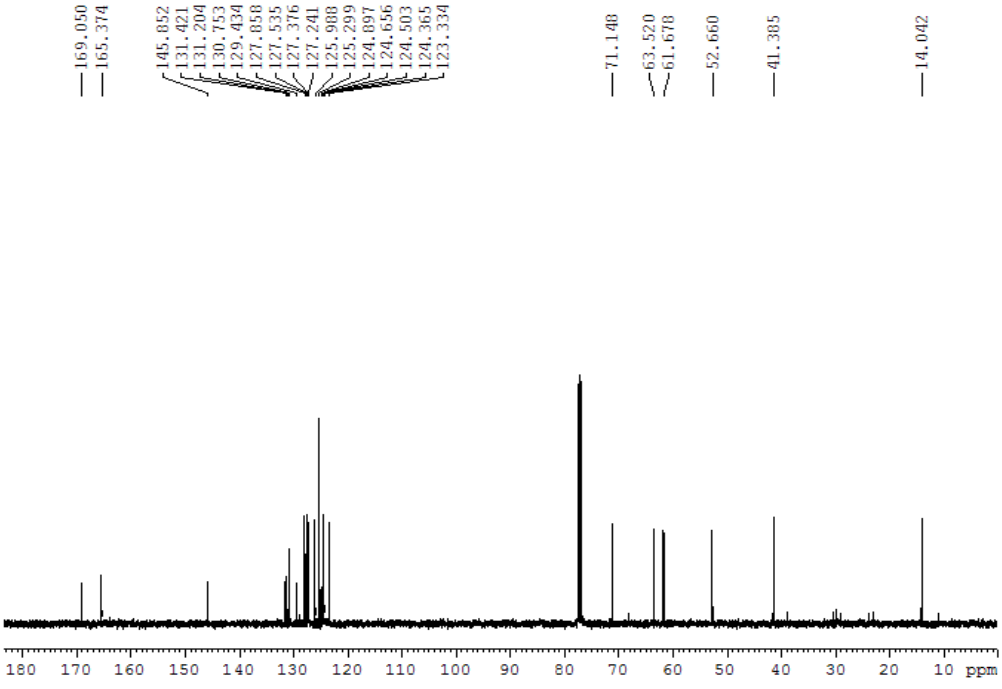
^{13}C NMR spectra of 3 (C*D*Cl$_3$)



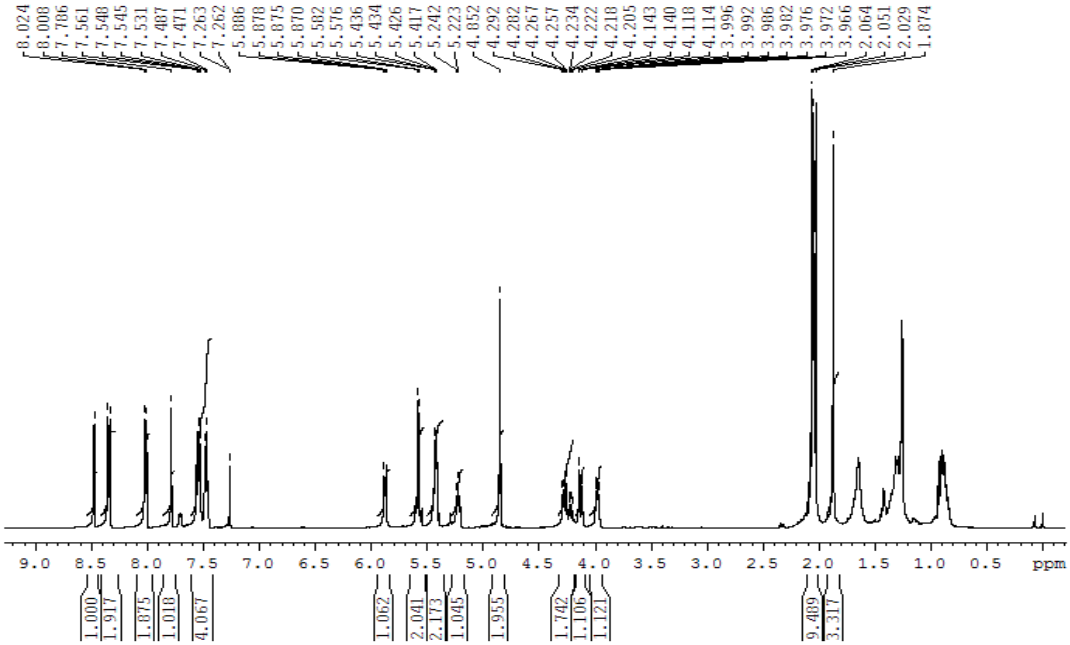
^{1}H NMR spectra of 4 (C*D*Cl$_3$)



^{13}C NMR spectra of 4 (C*D*Cl$_3$)



^{1}H NMR spectra of 5 (C*D*Cl$_3$)



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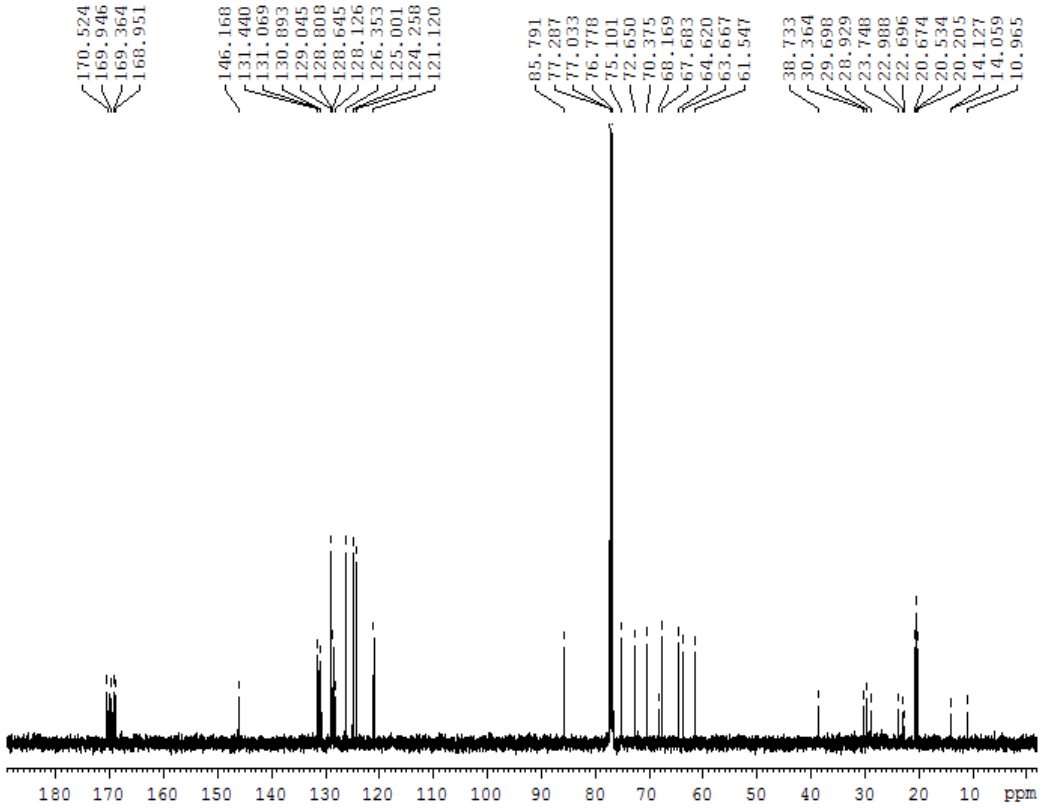
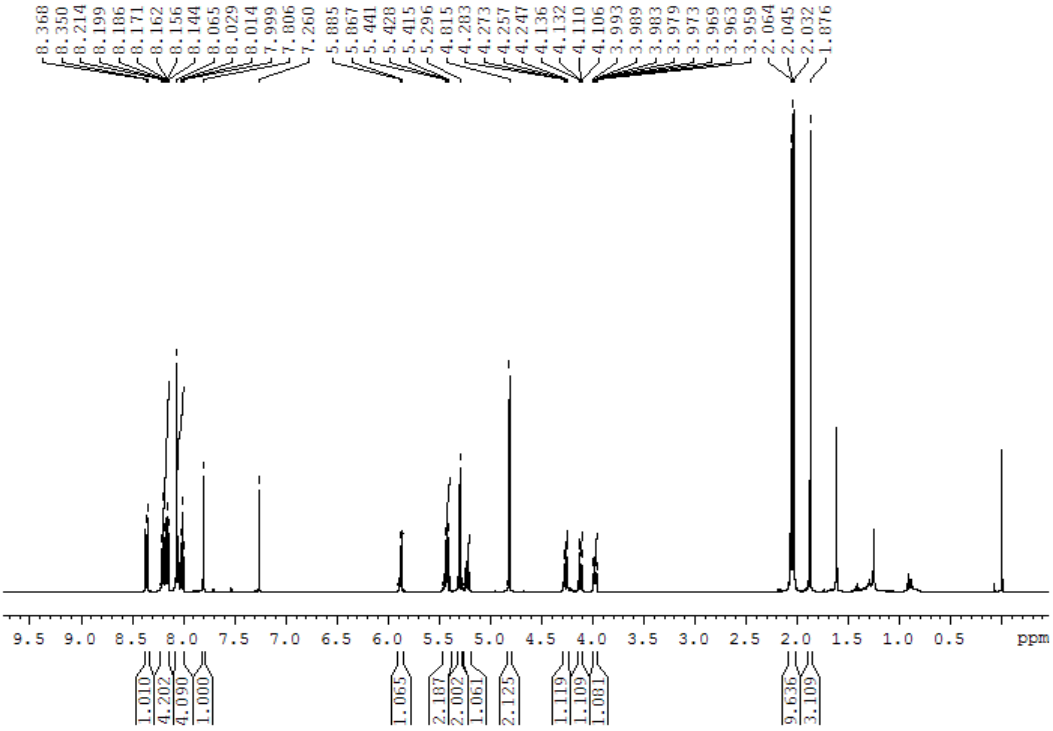


^{1}H NMR spectra of 6 (C*D*Cl$_3$)



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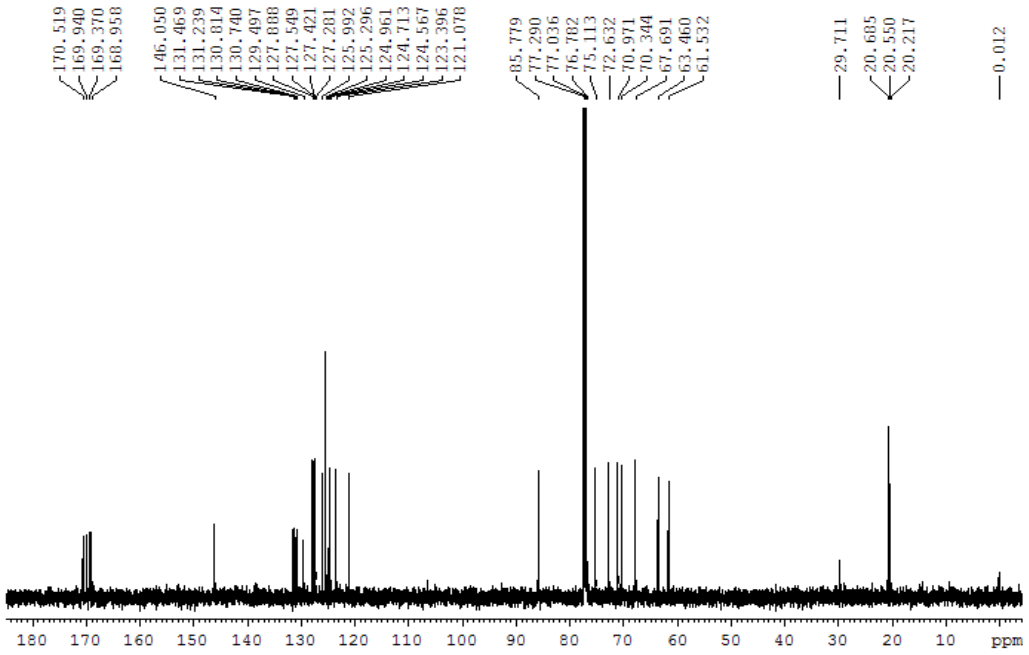
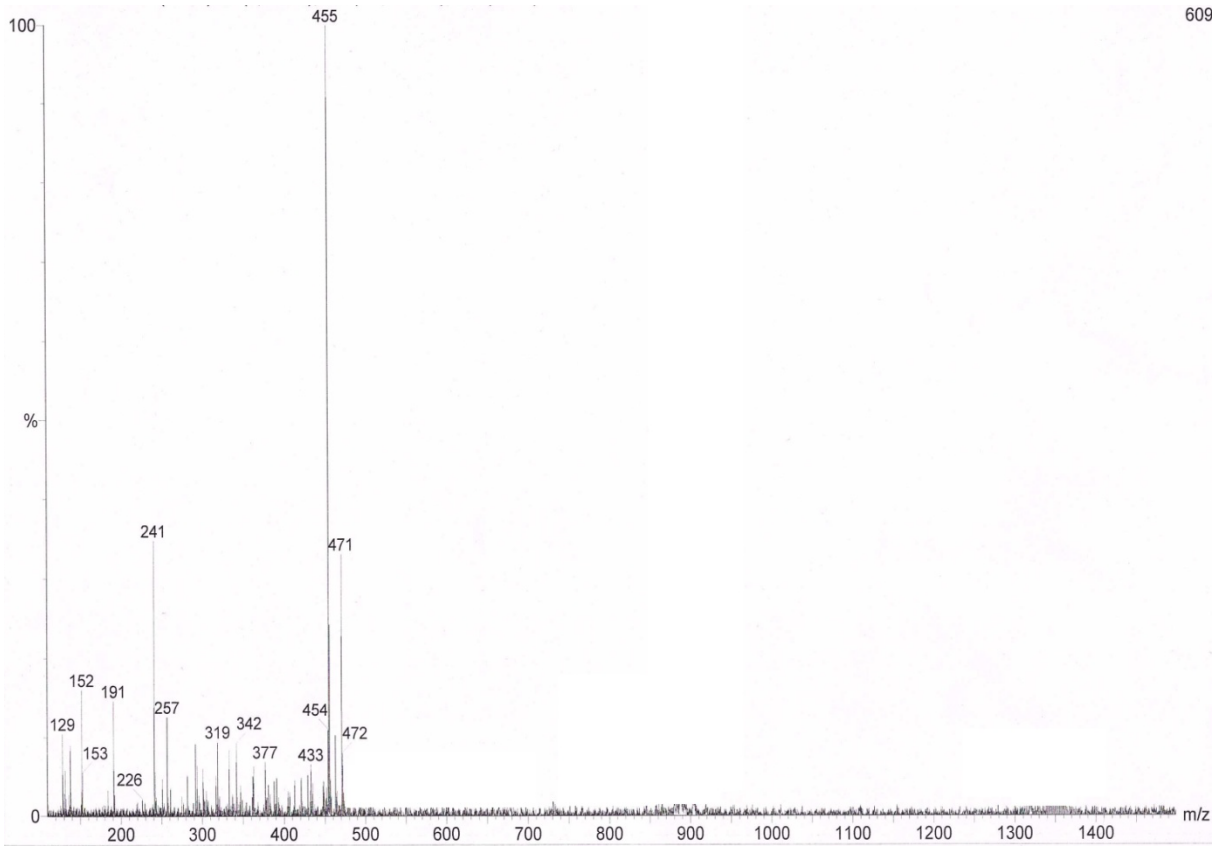
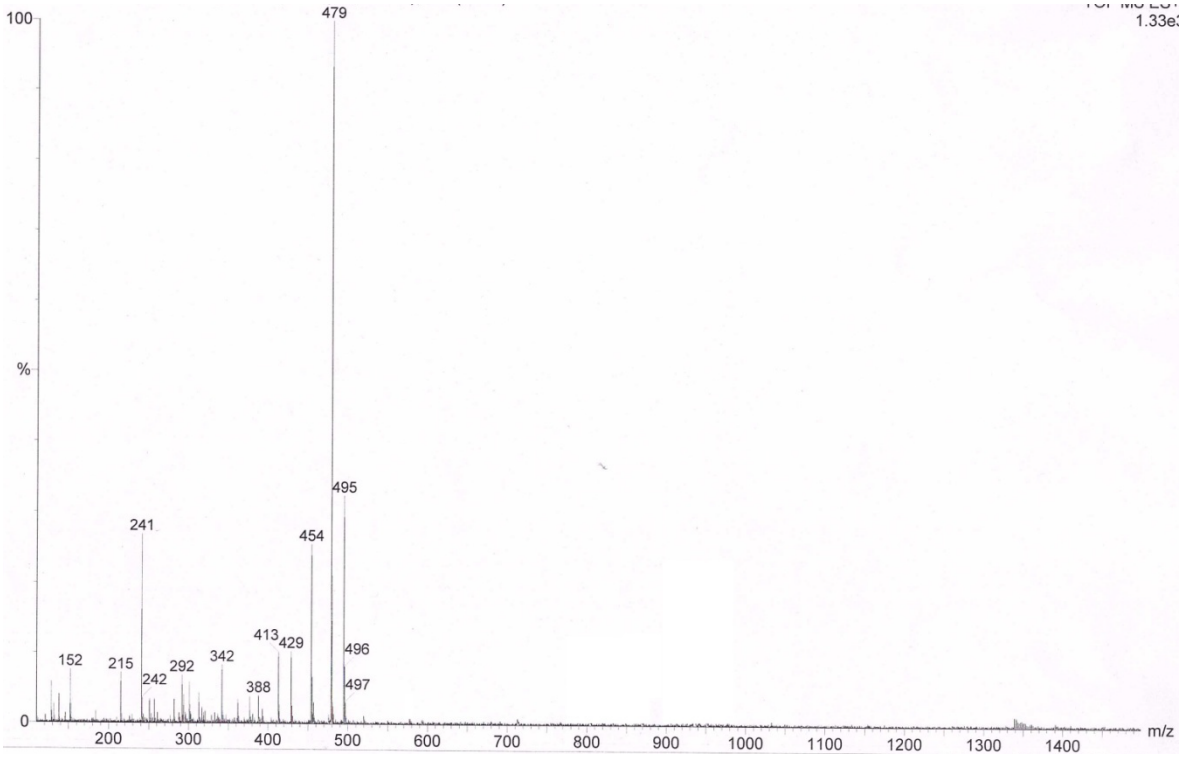
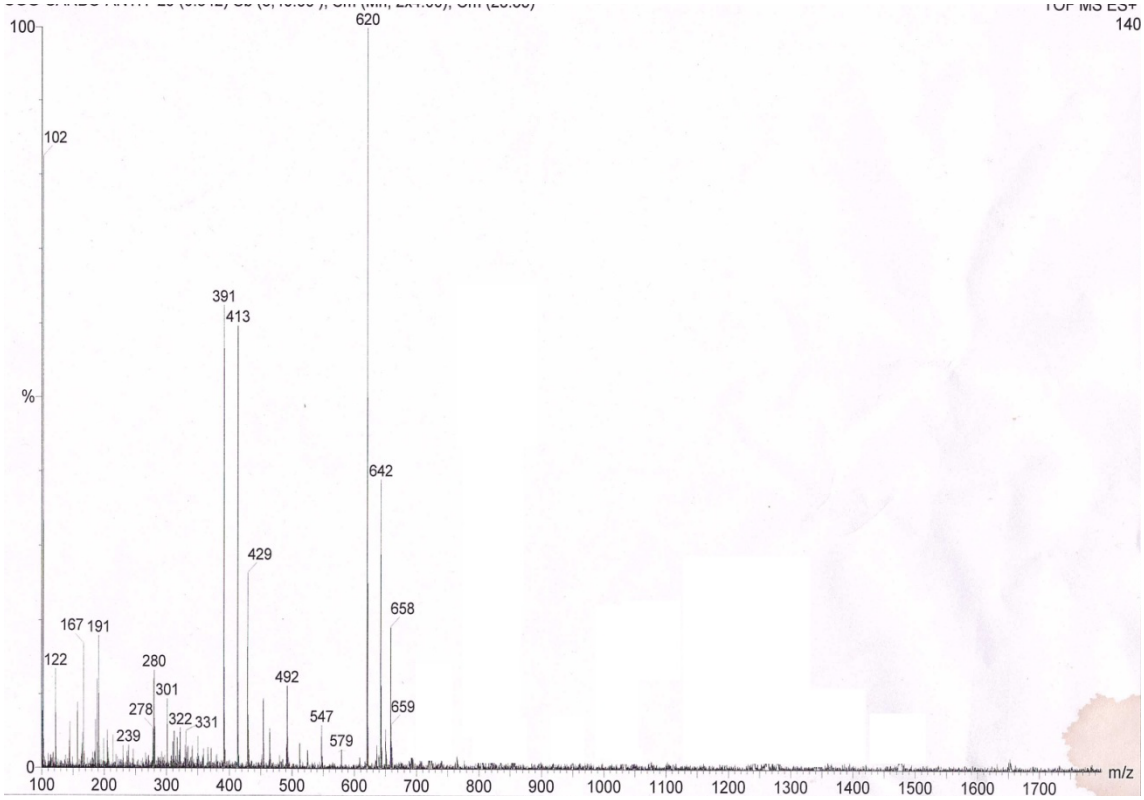




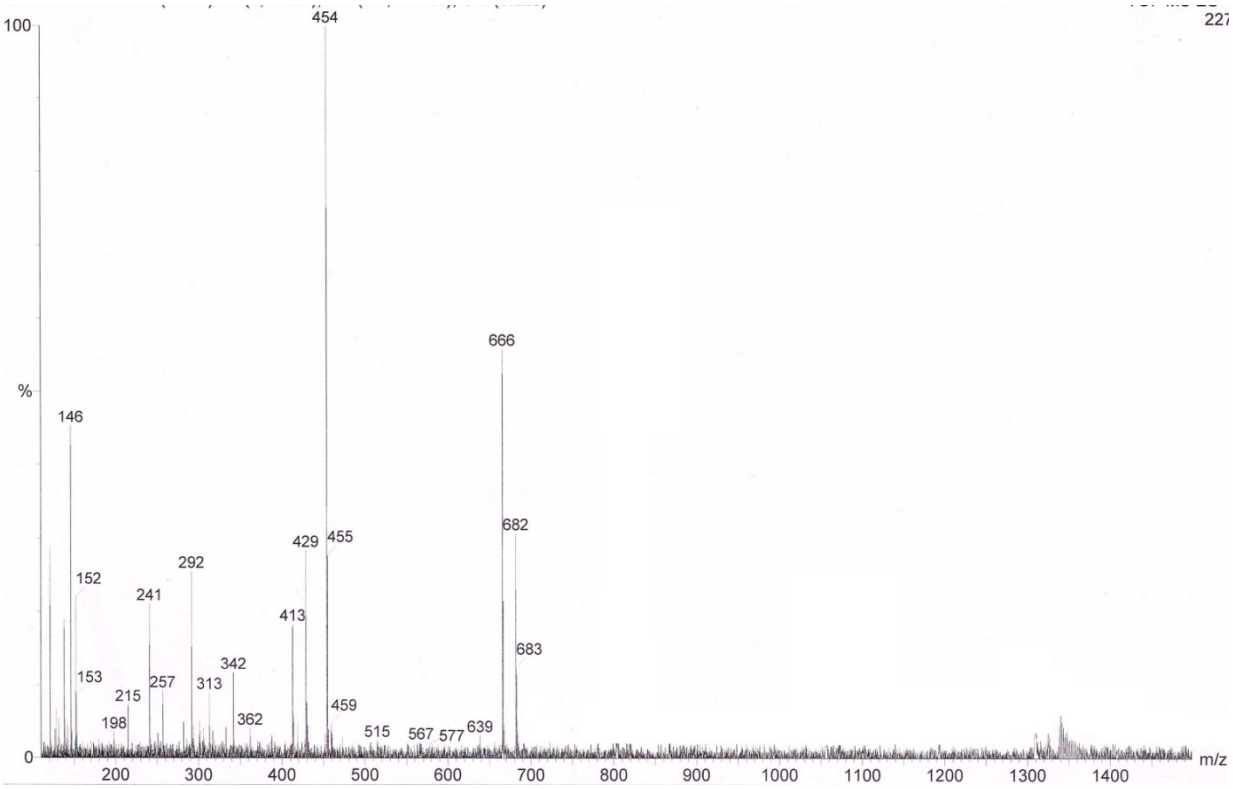
Electospray mass spectrum of **3**.



Electospray mass spectrum of **4**.



Electospray mass spectrum of **5**



Electospray mass spectrum of **6**.

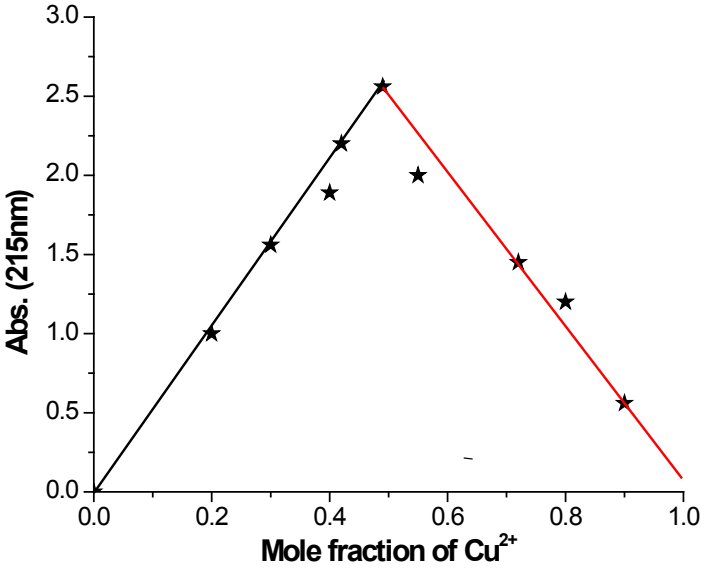


Figure S1. Job's plot of **4** with Cu^{2+} in CH_3CN indicating the formation of 1:1 complex species.

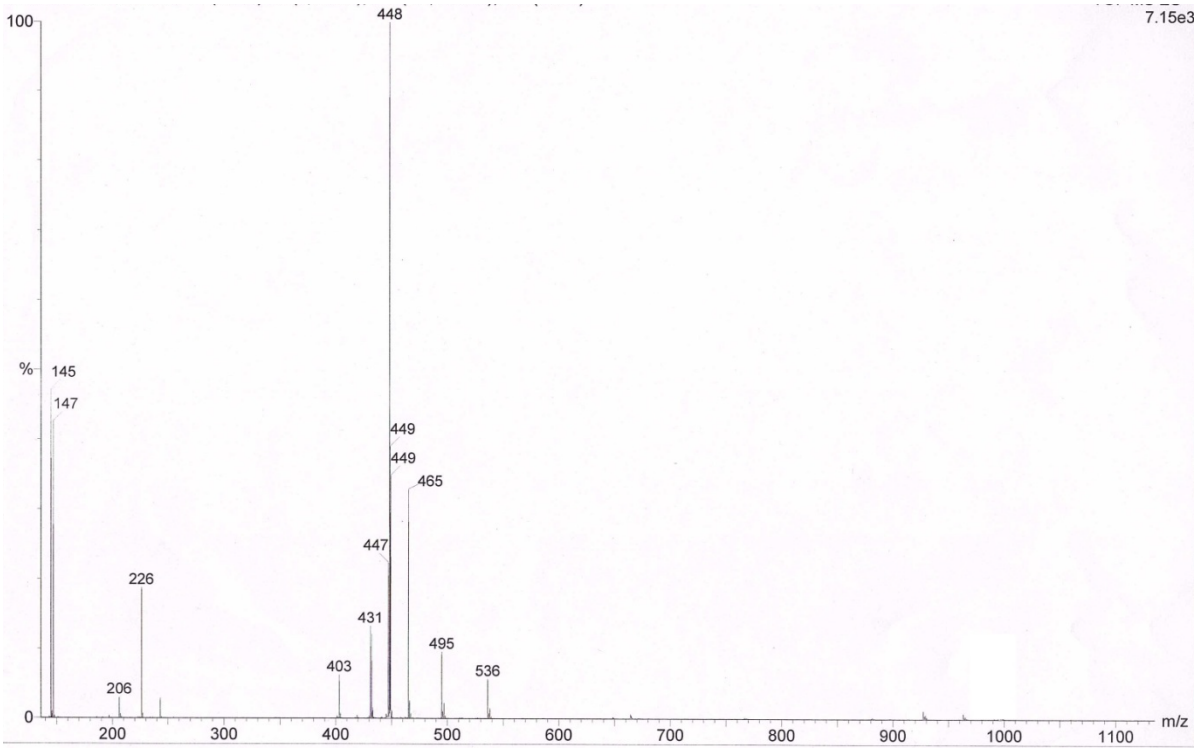


Figure S2. Electospray mass spectrum of [**3.**Cu^{2+}]

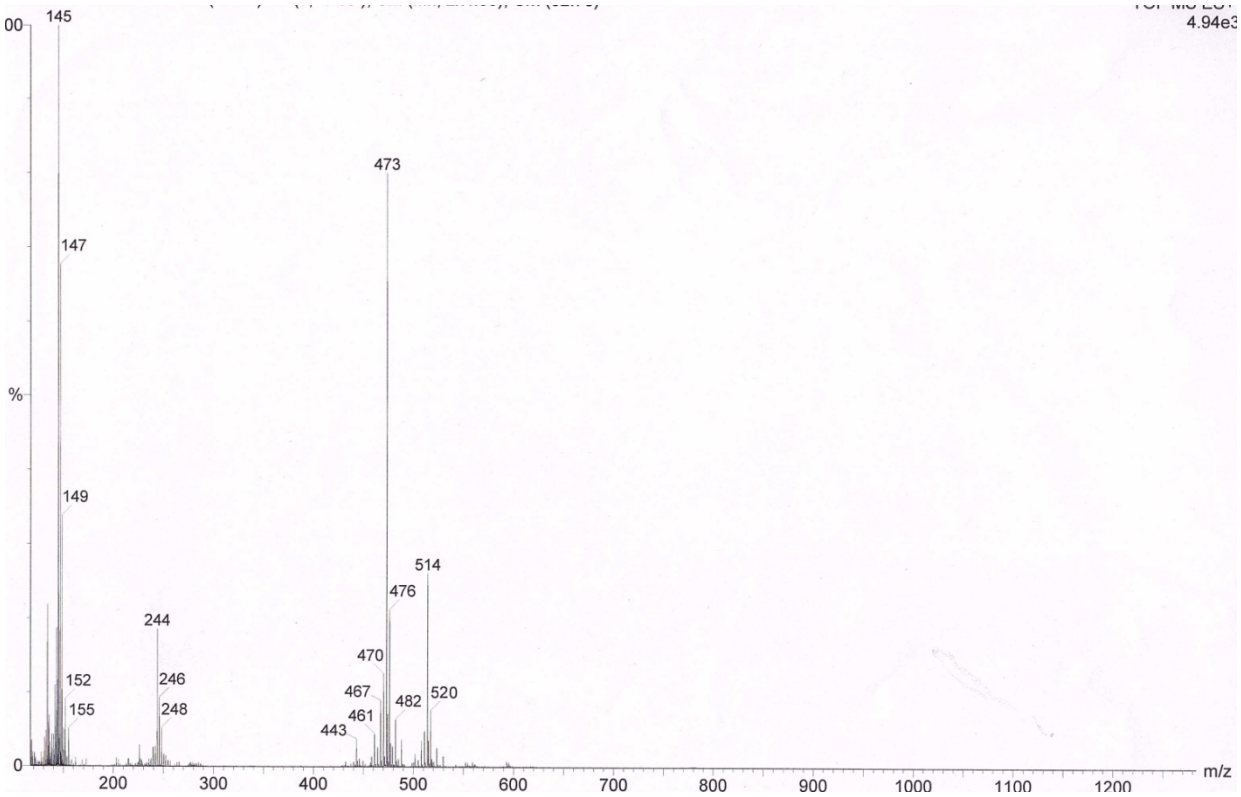


Figure S3. Electospray mass spectrum of [**4.**Cu^{2+}]

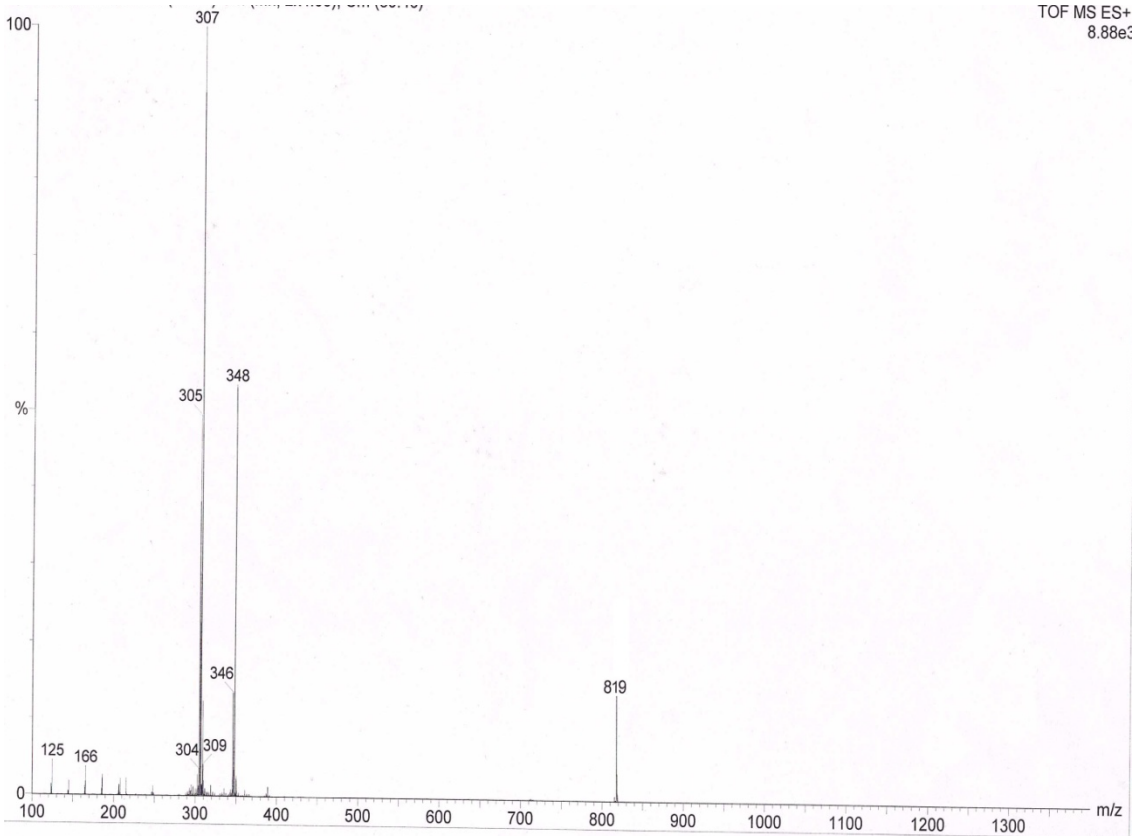


Figure S4. Electospray mass spectrum of [**5.**Hg^{2+}]

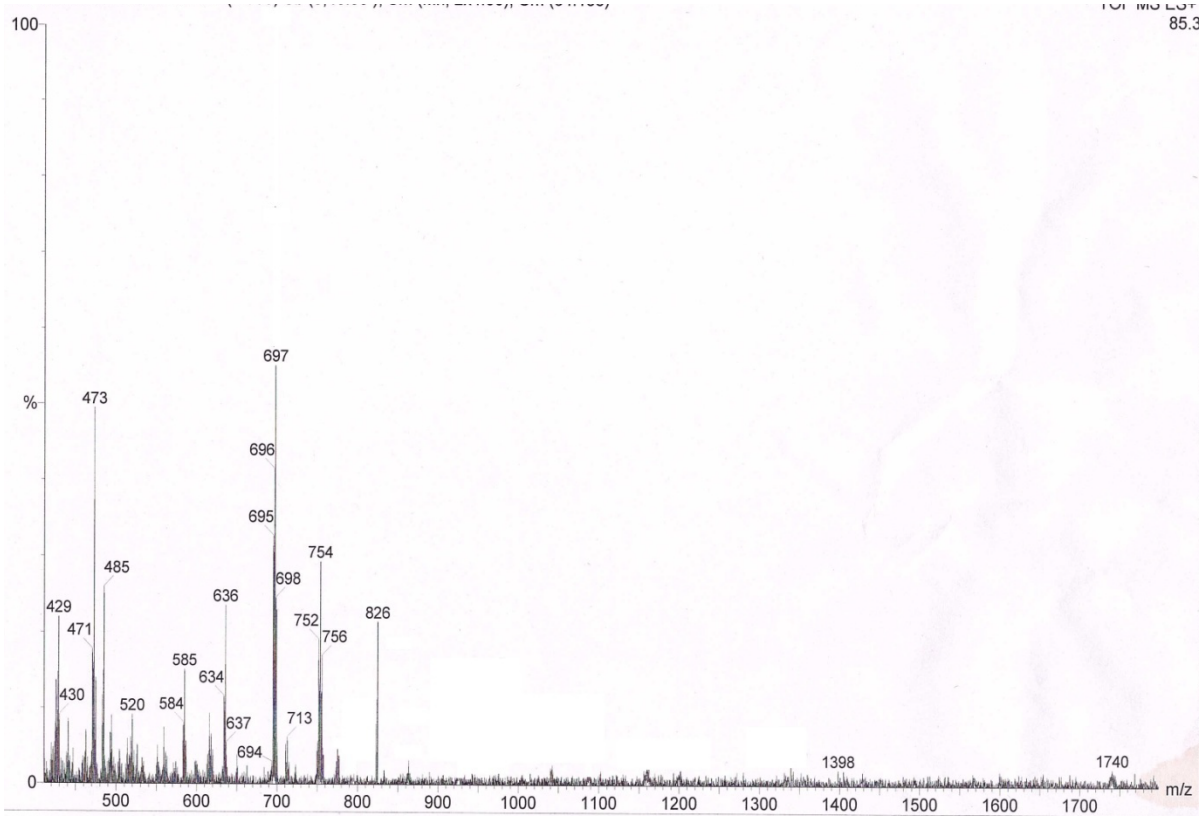


Figure S5. Electospray mass spectrum of [**5**.Pb^{2+}]

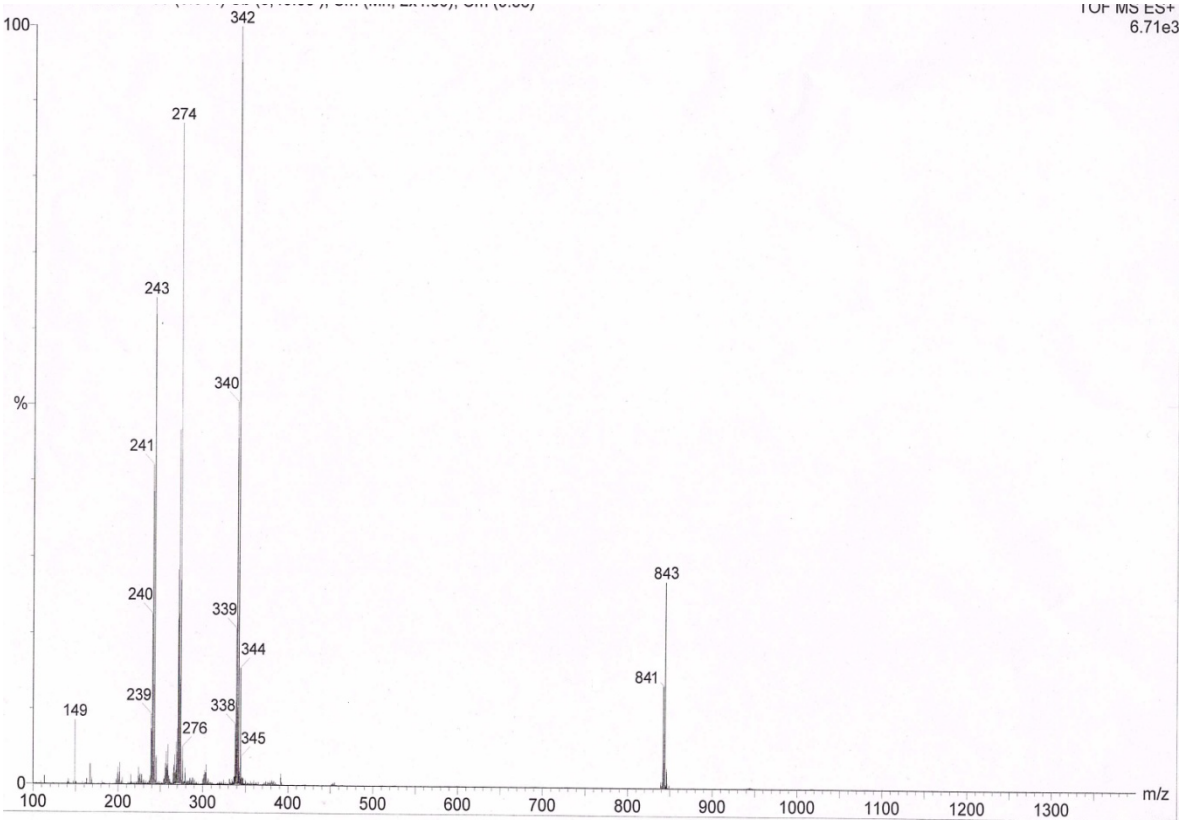


Figure S6. Electospray mass spectrum of [**6.**Hg^{2+}]

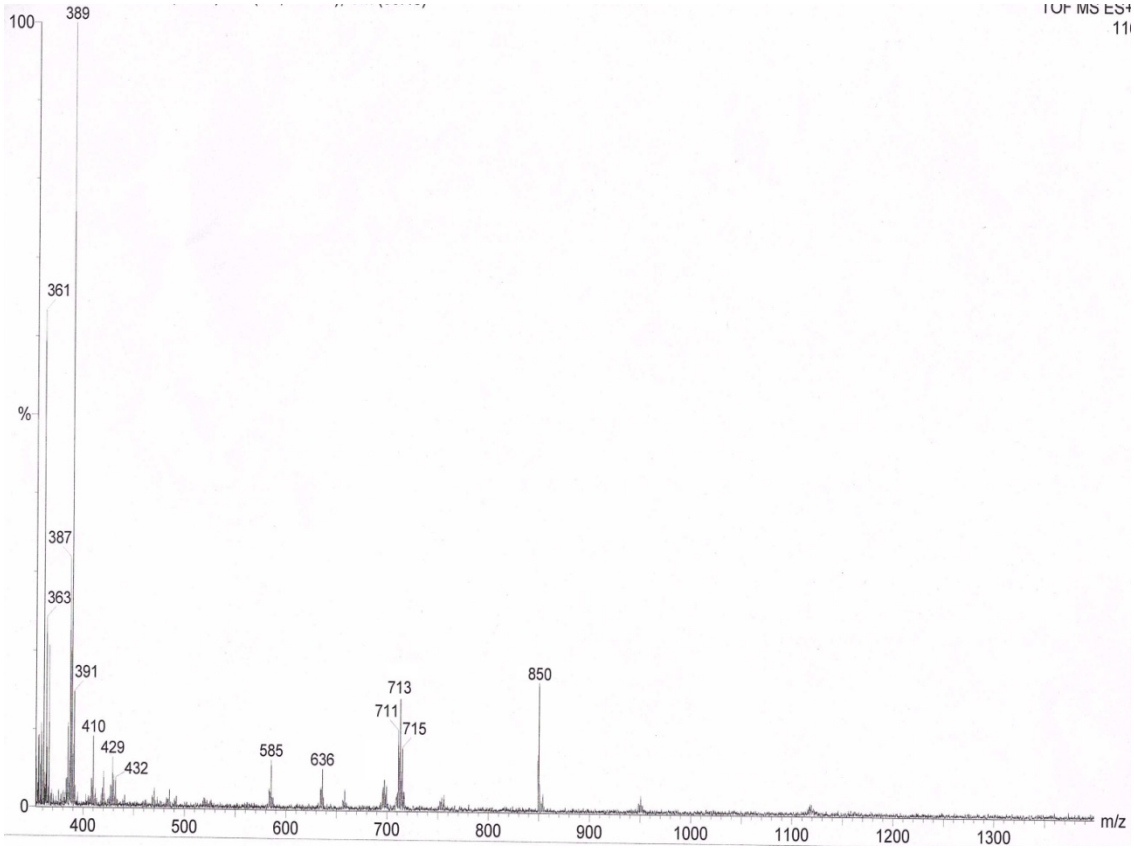


Figure S7. Electospray mass spectrum of [**6.**Pb^{2+}]

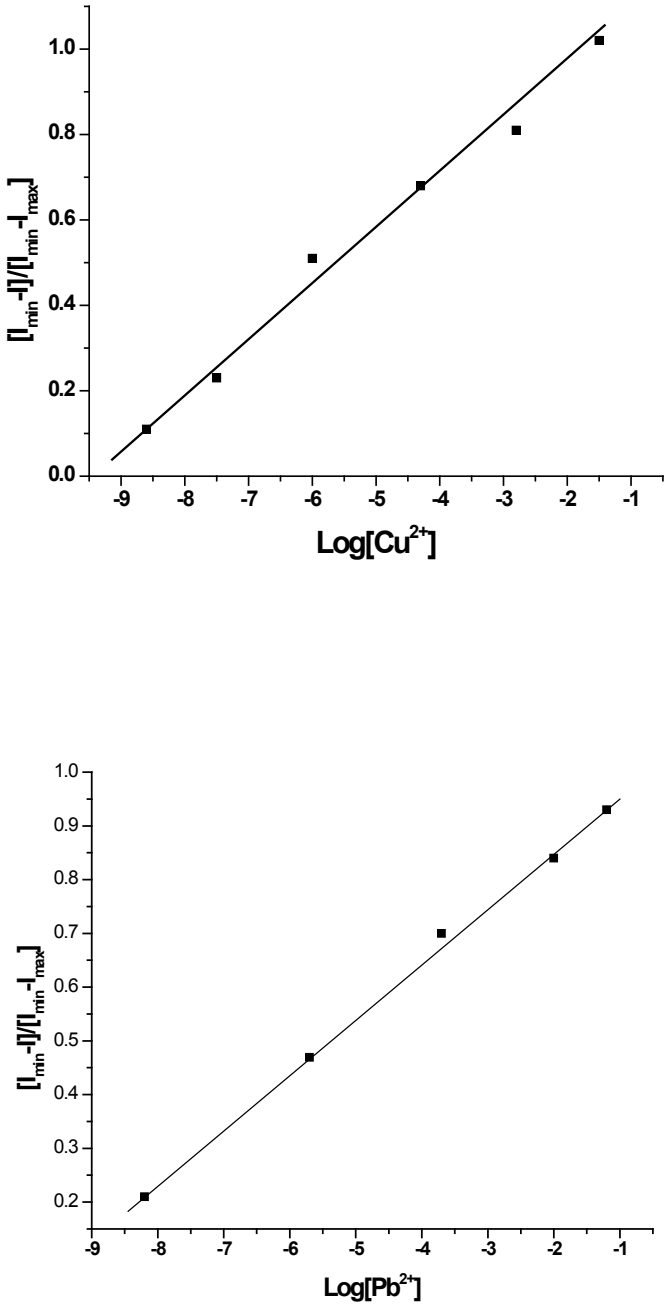


Figure S8. Fluorescence intensity of **3** or **4** at each concentration of Cu^{2+} added (top), and of **6** at each concentration of Pb^{2+} (bottom) normalized between the minimum fluorescence intensity and the maximum fluorescence intensity.

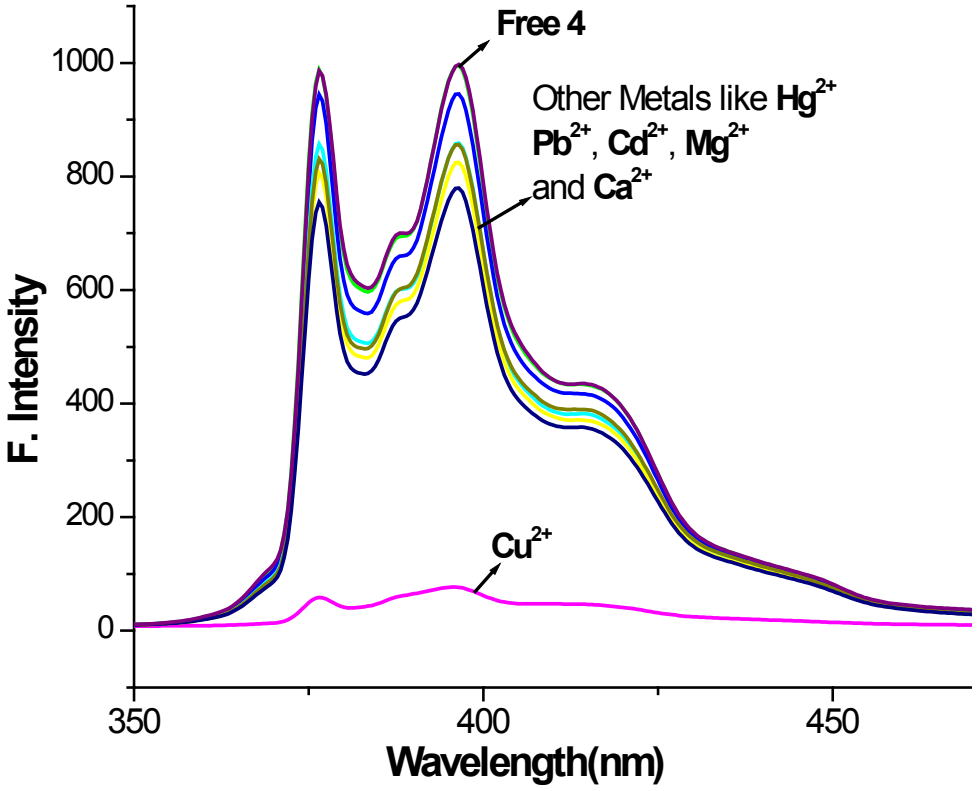


Figure S9. Fluorescene emission changes of **4** (1.5 x10^{-10} M) upon addition of several cations upto 1 equivalent in CH_3CN/H_2O (2:8) solution.

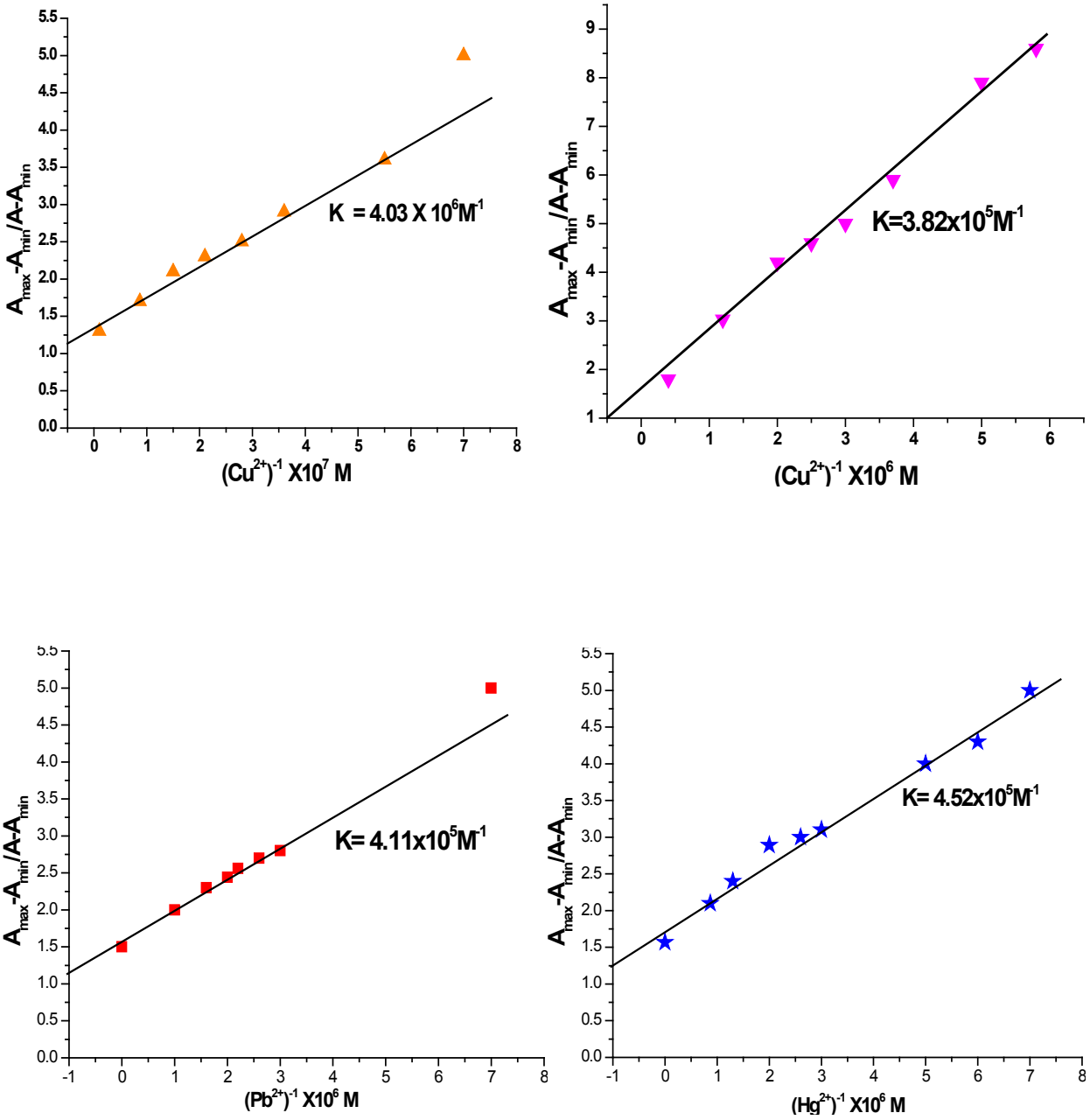


Figure S10. Quantitative binding data (Benesi-Hildebrand plot) for **3** and **4** with Cu^{2+} and **6** with Pb^{2+} and Hg^{2+}ion.

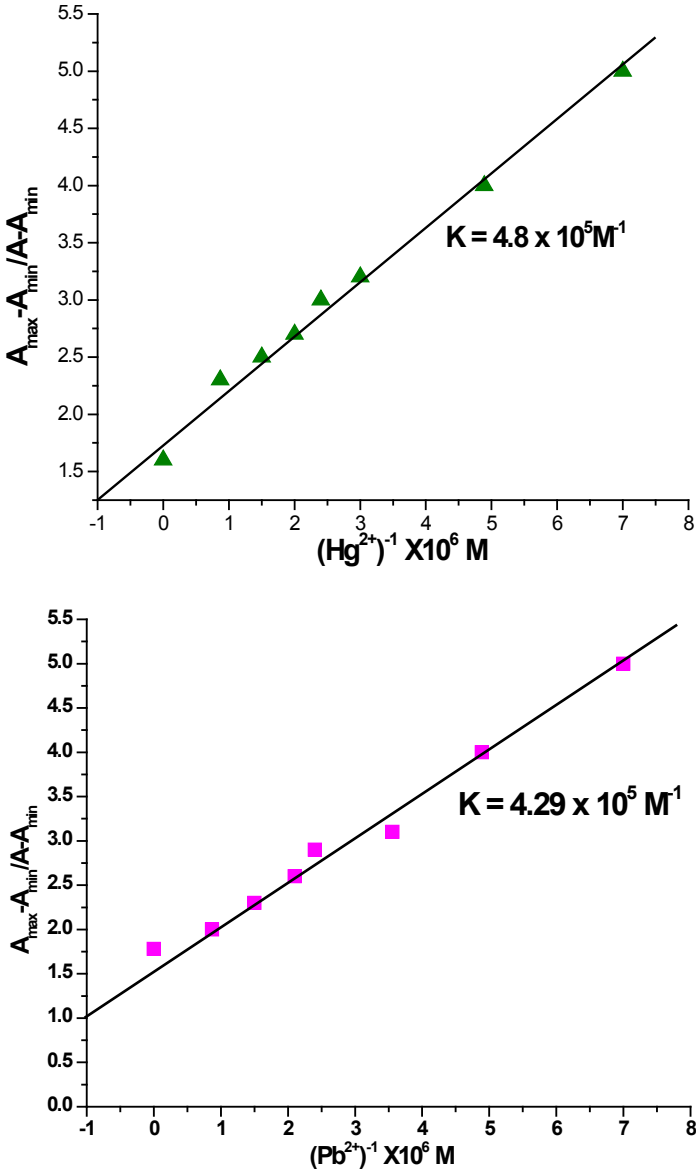


Figure S11. Quantitative binding data (Benesi-Hildebrand plot) for **5** with Hg^{2+} and Pb^{2+}ion.

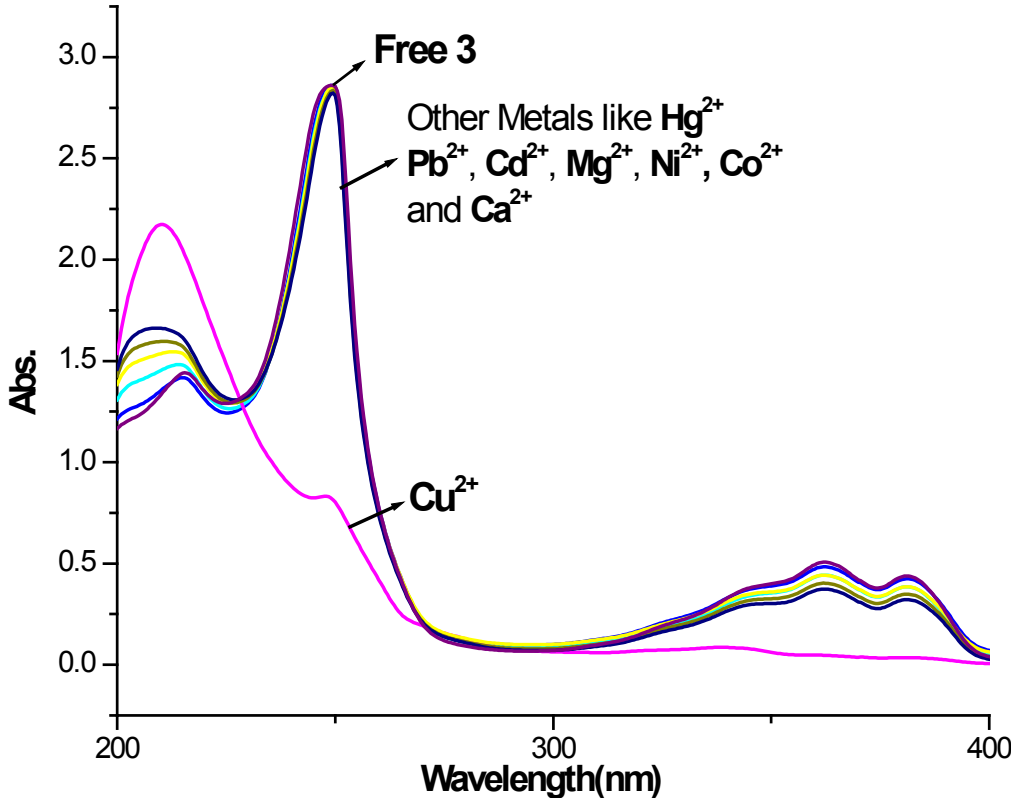


Figure S12: Changes in the absorption spectra of **3** (1 x 10^{-5} M) in CH_3CN/H_2O (2:8) upon addition of several metal cations tested.

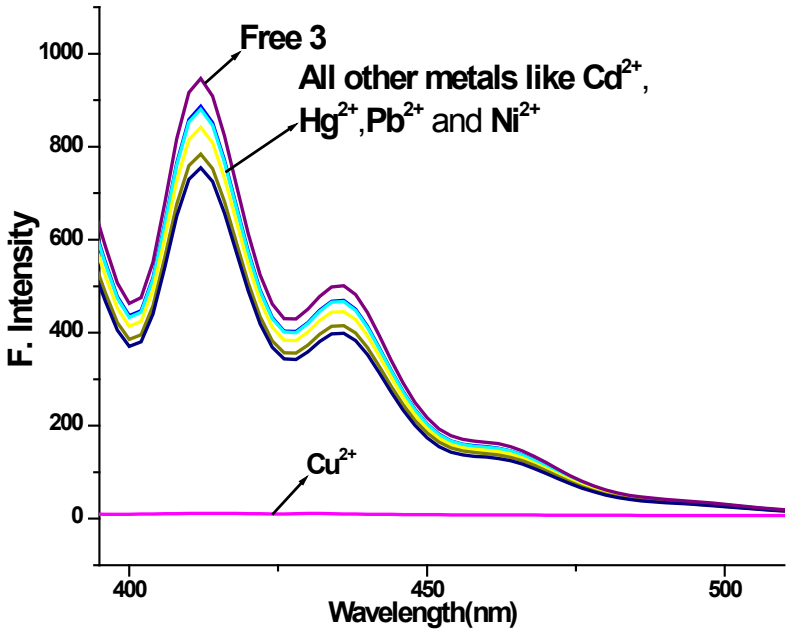


Figure S13. Fluorescene emission changes of **3** (1.5×10^{-10} M) upon addition of several cations upto 1 equivalent in CH_3CN/H_2O (2:8) solution.

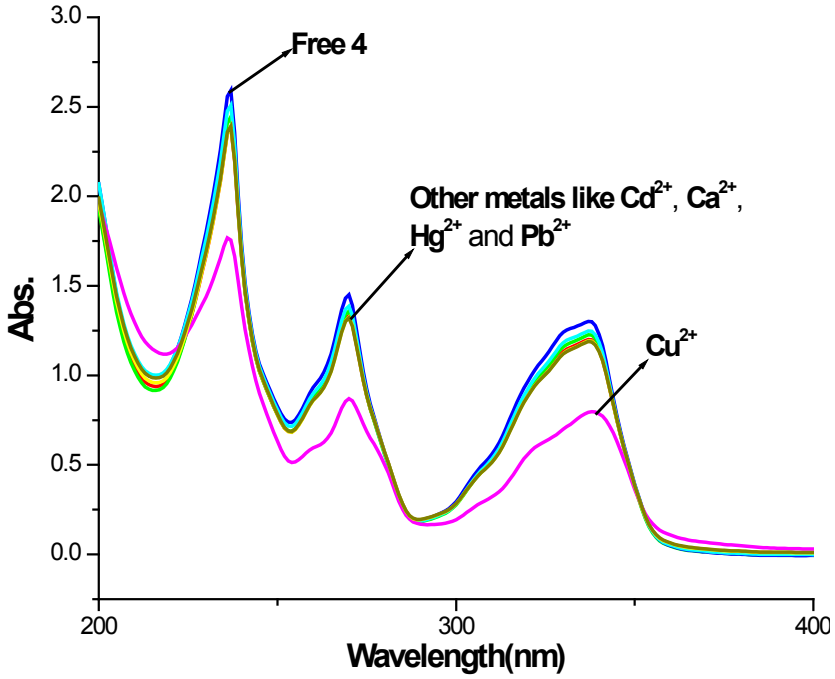


Figure S14. Changes in the absorption spectra of **4** (1 x 10^{-5} M) in CH_3CN/H_2O (2:8) upon addition of several metal cations tested.

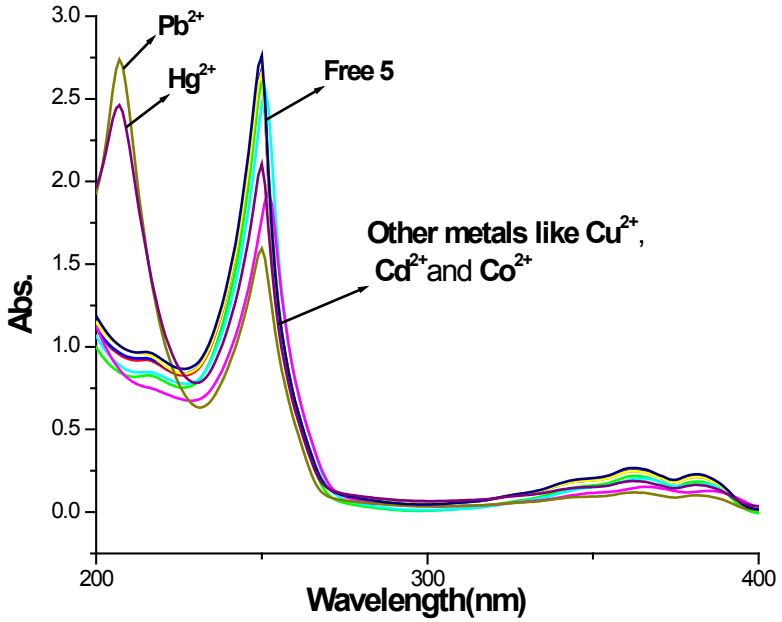


Figure S15. Changes in the absorption spectra of **5** (1 x 10^{-5} M) in CH_3CN/H_2O (2:8) upon addition of several metal cations tested.

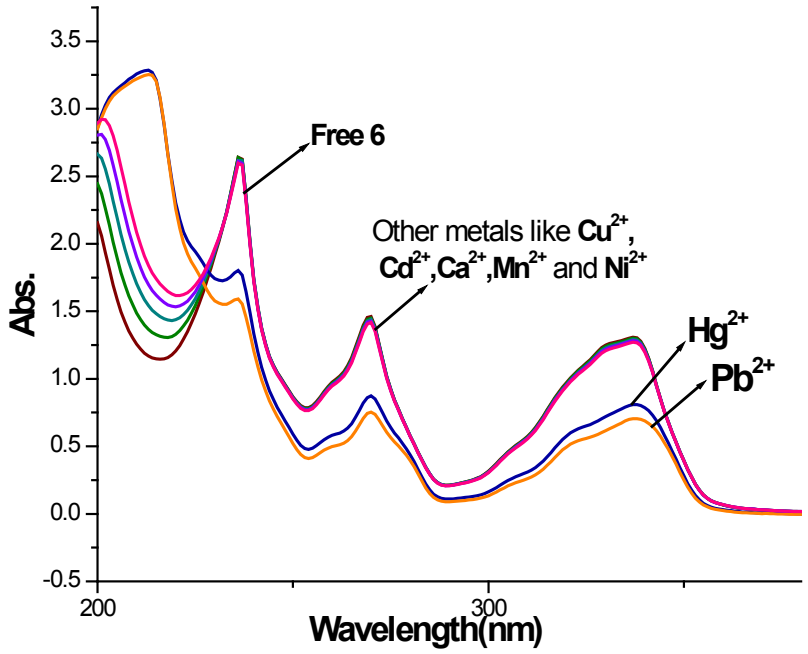


Figure S16. Changes in the absorption spectra of **6** (1 x 10^{-5} M) in CH_3CN/H_2O (2:8) upon addition of several metal cations tested.

Computational details

Calculated geometries were fully optimized in the gas-phase with tight convergence criteria at the DFT level with the Gaussian 09 package[1] using the Cam-B3LYP[2] functional to produce a better performance where weak interactions are involved, such as those between ligands and heavy metals. The 6–31G* basis set was used in the optimizations for all atoms and the LANL2DZ[3] basis set with effective core potentials for Pb, Hg and Cu. The LANL2DZ basis set uses the effective core potentials of Hay and Wadt. The nature of the optimized stationary points was confirmed by analytic computation of harmonic force constants at the aforementioned DFT level. From these gas-phase optimized geometries, all reported data were obtained by means of single point (SP) calculations, at the same level of theory. Bond orders were characterized by the Wiberg bond index (WBI)[4] and calculated with the Natural Bond Orbital (NBO) population analysis, as the sum of squares of the off-diagonal density matrix elements between atoms.

Cartesian coordinates for the calculated structure of ligand **3** (in Å).

C	-2.61011800	4.05303800	0.80185300	H	-1.43449600	-2.06542100	2.56094300
C	-3.73617300	3.79894600	0.08320600	H	-2.09319700	-3.29568600	1.47305500
C	-4.26308700	2.47469200	-0.01491000	C	-0.19755300	-2.52660600	0.87293600
C	-3.60155700	1.40134900	0.66534400	C	0.50269000	-1.66593300	0.06840300
C	-2.41073500	1.71412700	1.39684100	N	1.65325300	-2.32830100	-0.18870700
C	-1.93557500	2.98868500	1.46248800	H	0.29543200	-0.67839900	-0.30591800
C	-5.40915500	2.20535600	-0.75747300	N	0.54662000	-3.64736700	1.06216700
C	-4.12702400	0.09624200	0.59603100	N	1.66615100	-3.52720100	0.42091200
C	-5.26138500	-0.16921300	-0.19402600	C	2.77922900	-1.94475900	-1.00487700
C	-5.91654000	0.91569600	-0.87248900	H	3.46699700	-2.79153900	-0.98801500
C	-7.08166900	0.65530100	-1.65889800	H	2.45177400	-1.78663700	-2.03810700
H	-7.56123200	1.49494900	-2.15431700	C	3.42909900	-0.65208200	-0.51532900
C	-7.57443100	-0.60388800	-1.79086200	O	2.76930000	0.29254400	-0.11581400
C	-6.92022700	-1.68800200	-1.14168600	N	4.77486800	-0.61770400	-0.61803400
C	-5.81442400	-1.47977900	-0.37594700	H	5.32514900	-1.42209300	-0.89074400
H	-5.91605900	3.02144300	-1.26667700	C	5.51632700	0.56149500	-0.25299300
H	-2.21582800	5.06218900	0.86851500	H	5.21736500	1.42499800	-0.85705200
H	-4.25773600	4.59854600	-0.43553700	H	5.33836900	0.83975100	0.79189300
H	-1.85851900	0.91301700	1.87161700	C	6.98764700	0.28384400	-0.45738600
H	-1.02505600	3.19677100	2.01572000	O	7.42606200	-0.77578100	-0.84335800
H	-8.45821100	-0.79079300	-2.39257600	O	7.72830200	1.34634400	-0.15733900
H	-7.30718600	-2.69477700	-1.26518800	C	9.15465200	1.18886900	-0.30997400
H	-5.33230900	-2.33313300	0.08412200	H	9.48320000	0.36705500	0.33144500
C	-3.45416800	-0.98882100	1.39681600	H	9.36378600	0.90776600	-1.34529500
H	-4.08794400	-1.87744800	1.48571000	C	9.79620100	2.50318500	0.06842500
H	-3.27603100	-0.63514200	2.42384700	H	9.56361900	2.76675700	1.10340800
O	-2.22080500	-1.33433500	0.79358900	H	10.88246400	2.42686900	-0.03241300
C	-1.53848700	-2.34584700	1.49976100	H	9.44531200	3.30940000	-0.58094300

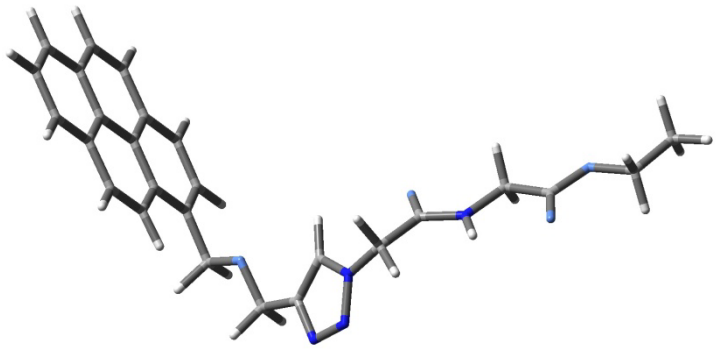


Figure S17. Calculated (cam-B3LYP/6–31G*/LANL2DZecp) structure of **4.**

Cartesian coordinates for the calculated structure of **4** (in Å).

N	2.54512200	3.26999000	-1.11437100	C	7.45064000	-1.07310100	-0.25885700
N	1.55618300	3.86585200	-0.52595700	C	-3.91337300	0.62942700	0.53315700
N	2.38111600	1.94711700	-0.93491300	C	-3.53038500	0.51571700	2.91604300
C	0.74638700	2.93262100	0.03882100	O	7.88469500	-0.44594500	-1.19816400
C	1.26486800	1.68981700	-0.21623500	O	8.16767400	-1.89781300	0.49817700
C	3.33443200	1.03639400	-1.52208600	C	-4.74097300	-0.52069700	0.63113900
C	-0.47485300	3.30135700	0.81107100	C	-3.72496700	1.22488400	-0.76453500
H	0.95966100	0.69542400	0.05946400	C	-4.33028700	-0.61283900	3.01835700
H	2.83303100	0.39776500	-2.25732600	H	-3.05991000	0.91860700	3.80848100
H	4.06220800	1.65788400	-2.04586100	C	9.56197200	-2.02833800	0.15001400
C	3.97960400	0.12913900	-0.47667800	C	-5.37443300	-1.05211400	-0.53339300
H	-0.98396200	4.14492500	0.32079500	C	-4.94854600	-1.14691400	1.88892500
H	-0.20606900	3.63524600	1.82635700	C	-4.32920200	0.72220500	-1.86475700
O	-1.30998500	2.16744300	0.87976200	H	-3.05671800	2.07253800	-0.85189500
O	3.33523900	-0.37146300	0.42980200	H	-4.48109500	-1.08782300	3.98348300
N	5.29210800	-0.12046200	-0.67000700	H	9.63025600	-2.37702800	-0.88365100
C	-2.47319900	2.39515400	1.65148000	H	10.02575200	-1.03983200	0.19974100
H	5.83914200	0.34015100	-1.38607400	C	10.18057500	-3.00179600	1.12572200
C	6.01307900	-1.01059400	0.20270300	C	-5.17943400	-0.43297500	-1.79421300
C	-3.31545000	1.14896800	1.69672400	C	-6.20415400	-2.20010800	-0.43474500
H	-2.19395000	2.69007400	2.67382200	C	-5.79144900	-2.31064800	1.95779900
H	-3.04290000	3.23343200	1.21869900	H	-4.17178900	1.18525300	-2.83492000
H	5.57962200	-2.01654300	0.19422800	H	9.69431000	-3.97871600	1.06282600
H	5.97741000	-0.66846700	1.24313500	H	11.24245700	-3.12949600	0.89755800

H	10.08978300	-2.63577400	2.15164000	C	-6.62048300	-2.08693800	-2.81733100
C	-5.81046200	-0.96525800	-2.92206400	H	-5.65867200	-0.48895900	-3.88657300
C	-6.81593100	-2.69974100	-1.58625000	H	-7.45085700	-3.57786800	-1.50885600
C	-6.38813000	-2.81154800	0.85430100	H	-7.02312500	-3.69054900	0.92018100
H	-5.93818500	-2.77965200	2.92664400	H	-7.10416000	-2.48828600	-3.70246600

Cartesian coordinates for the calculated structure of **3.**$Cu(ClO_4)_2$.

N	0.70661800	-1.30095800	0.21626500	H	7.11834100	5.89523600	-2.60983700
N	-0.27276600	-2.09569100	-0.06959000	H	7.55061400	7.12212100	-1.40432500
N	0.22091000	-0.07616900	0.47090800	H	7.95393400	5.41871300	-1.11911800
C	-1.42180400	-1.39613500	0.01142700	Cu	2.71445000	-1.63059000	-0.05523700
C	-1.12229100	-0.09876900	0.35935500	Cl	4.70511100	-0.67226200	1.80197900
C	1.08091100	1.00772600	0.91175300	O	5.21953300	0.65656300	1.44412600
C	-2.76435100	-1.99318100	-0.24960100	O	5.54044500	-1.34177000	2.78088200
H	-1.75021600	0.76002700	0.53180500	O	3.28707400	-0.55835800	2.26385900
H	0.46799000	1.90679200	0.98365000	O	4.63260300	-1.53053400	0.53217900
H	1.49333000	0.76851200	1.89687500	Cl	2.64156200	-4.03417200	-1.36467700
C	2.26533700	1.21256300	-0.01748200	O	3.82257700	-4.85556500	-1.55588600
H	-2.95160300	-2.82110700	0.45118000	O	2.75216300	-2.71824000	-2.08085400
H	-2.79873500	-2.41481300	-1.26535600	O	1.40732600	-4.72505600	-1.69612700
O	-3.70342600	-0.96067100	-0.08864200	O	2.57990400	-3.57012600	0.12102000
O	2.80694600	0.26168300	-0.61181000	C	-5.97728800	-0.22872200	-0.08816800
N	2.73760000	2.44056300	-0.12692900	C	-6.24829300	0.20227200	1.22556900
C	-5.04300200	-1.39292100	-0.28333100	C	-6.57320000	0.42036500	-1.18651500
H	2.32247600	3.23319500	0.35544400	C	-7.18697400	1.26213900	1.44795600
C	4.00723500	2.72323400	-0.77021600	C	-5.61763100	-0.37468300	2.37498200
H	-5.14677500	-1.83410100	-1.27965400	C	-7.51251500	1.48249600	-0.95058800
H	-5.27704300	-2.19077900	0.43526000	C	-6.29373800	0.08865000	-2.55332400
H	3.95642500	2.53845300	-1.84719300	C	-7.47589800	1.67685500	2.78450800
H	4.78702300	2.07857800	-0.35238500	C	-7.80131800	1.86713400	0.35483500
C	4.31771700	4.18009300	-0.50587700	C	-5.91599700	0.05046700	3.63439300
O	3.58506800	4.90412700	0.13356800	H	-4.86593900	-1.14198500	2.23697900
O	5.46318600	4.54156700	-1.05569000	C	-8.13741600	2.13219200	-2.06036600
C	5.87218500	5.91324600	-0.84835800	C	-6.90301600	0.73787700	-3.58344400
H	5.09824000	6.56775800	-1.25713300	H	-5.56647300	-0.68048200	-2.78174300
H	5.93287200	6.09338400	0.22760900	C	-6.86498900	1.08922900	3.84814500
C	7.20369100	6.09376100	-1.53838500	H	-8.19654800	2.47675400	2.92922600

H	-8.51982700	2.66510500	0.52489100	H	-6.66383000	0.46609200	-4.60681500
H	-5.42120300	-0.40217700	4.48812200	H	-7.09086600	1.41052100	4.85986500
H	-8.84986600	2.92557200	-1.85290100	H	-8.32630100	2.27390500	-4.17464200
C	-7.84772600	1.77379000	-3.33887500				

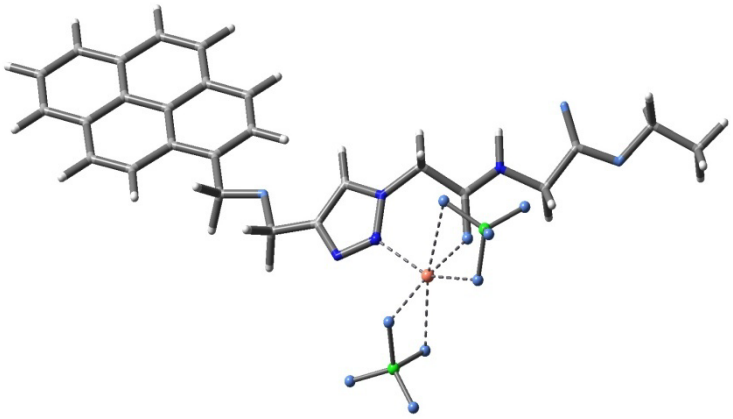


Figure S18. Calculated (cam-B3LYP/6–31G*/LANL2DZecp) structure for **4.**$Cu(ClO_4)_2$.

Cartesian coordinates for the calculated structure of **4.**$Cu(ClO_4)_2$.

N	1.52754100	-1.25534200	0.31260900	N	3.60492100	2.45928800	-0.02612600
N	0.52530300	-2.02670000	0.04443800	C	-4.22641600	-1.28509700	-0.04355300
N	1.07255200	-0.03073500	0.61673700	H	3.22150100	3.24704600	0.48947600
C	-0.60924600	-1.31281200	0.18877700	C	4.85520000	2.73732800	-0.70837500
C	-0.27459000	-0.03014700	0.55808500	C	-5.16748800	-0.10780100	-0.11642500
C	1.96752800	1.02960500	1.04602000	H	-4.37176100	-1.94413600	-0.91480300
C	-1.96451400	-1.90015100	-0.02421300	H	-4.43472800	-1.89036500	0.85212700
H	-0.87635800	0.83620100	0.77859600	H	4.76250900	2.58041100	-1.78698300
H	1.37341100	1.93663500	1.16184800	H	5.63839800	2.07013300	-0.33479200
H	2.41478800	0.76123400	2.00815400	C	5.19926700	4.18211400	-0.41972700
C	3.11817700	1.23636400	0.07542200	C	-6.55523800	-0.30909300	0.00116800
H	-2.18328800	-2.62901500	0.77115800	C	-4.67309400	1.17585400	-0.31486600
H	-1.99171700	-2.44317900	-0.97987800	O	4.50016600	4.90190800	0.26086000
O	-2.88737300	-0.84184000	-0.00388500	O	6.33206600	4.53803300	-0.99809500
O	3.62171400	0.29031500	-0.55878900	C	-7.42839000	0.80928900	-0.07198200

C	-7.13805600	-1.61318000	0.18983700
C	-5.52284700	2.27043800	-0.38808500
H	-3.60355300	1.31142600	-0.41626600
C	6.77173500	5.89727500	-0.77127400
C	-8.83999500	0.62947700	0.04940700
C	-6.90274300	2.11397600	-0.26687800
C	-8.47554400	-1.78170100	0.30305100
H	-6.49116700	-2.48235100	0.23813600
H	-5.11326800	3.26463300	-0.54318300
H	5.99839500	6.57445600	-1.14256800
H	6.86616600	6.05099700	0.30634300
C	8.08610200	6.07059600	-1.49509200
C	-9.37974200	-0.66829000	0.23973400
C	-9.71107000	1.74901400	-0.02073000
C	-7.80923000	3.22907200	-0.33525900
H	-8.89194600	-2.77500900	0.44438400
H	7.96690100	5.89854700	-2.56788400
H	8.45507900	7.08941100	-1.34772800
H	8.83569700	5.37315200	-1.11297700
C	-10.76386900	-0.82499600	0.35748500
C	-11.08785500	1.54895900	0.10213700
C	-9.14405800	3.05659400	-0.21747500
H	-7.39106600	4.22039800	-0.48507900
C	-11.60804400	0.27432800	0.28965300
H	-11.17338400	-1.82051000	0.50290600
H	-11.75298600	2.40613000	0.04878500
H	-9.81831100	3.90653300	-0.27053400
H	-12.68081400	0.13795900	0.38280200
Cu	3.52229100	-1.61143900	-0.03891400
Cl	5.58362800	-0.71939700	1.77446700
O	6.09731900	0.61328800	1.42982600
O	6.44528200	-1.41843300	2.70874600
O	4.18300800	-0.60421100	2.28666200
O	5.46003000	-1.54685300	0.48843800
Cl	3.36062600	-3.98746300	-1.38629100
O	4.52115200	-4.82077100	-1.63984300
O	3.46173500	-2.65895900	-2.08096300
O	2.10432200	-4.65461400	-1.68050800
O	3.36491600	-3.55036700	0.10915200

Cartesian coordinates for the calculated structure of **5**.

C	2.85163200	-1.33264500	-0.68567500
C	4.08633300	-0.93368200	0.11930300
C	4.40624600	0.55527400	-0.02286200
C	3.13919800	1.38826000	0.18745600
C	1.68828900	-0.35675500	-0.46209700
H	3.97948700	-1.13788000	1.18273200
H	3.10519400	-1.25003400	-1.74409900
H	2.79910600	1.26086000	1.22708700
H	1.28149700	-0.43000000	0.55456300
H	4.85408100	0.75341400	-0.99995000
O	2.13289300	0.95417900	-0.70995500
C	-0.73047600	-0.59840000	-1.11478100
C	-1.29787200	-0.84944600	-2.33160700
O	2.47201200	-2.69451600	-0.55410000
C	2.12798100	-3.38959100	0.56784100
O	1.72784400	-4.50999600	0.41443400
C	2.30751000	-2.79108300	1.94500400
H	3.36167300	-2.84394200	2.23569200
H	1.98392800	-1.75233600	2.02637900
H	1.72811700	-3.40186900	2.63641900
O	5.16126800	-1.71956300	-0.39258100
C	6.02735700	-2.26558500	0.48898800
O	5.90490400	-2.16809800	1.68786200
O	5.31188000	0.93994600	1.01600800
C	6.64532500	0.86578700	0.77130500
O	7.10679100	0.55709100	-0.29745700
C	7.14668800	-2.95396000	-0.22997500
H	7.72639100	-3.54692000	0.47615700

H	6.75766500	-3.58205900	-1.03390300	H	-4.45219900	1.78948000	-1.83724200
H	7.78273100	-2.18615700	-0.68116200	C	-6.62822600	2.91142800	1.17276900
C	7.42432400	1.17418000	2.01519700	C	-7.11293400	0.56230300	1.71357900
H	7.35441500	0.30905000	2.68228600	C	-7.59009000	-1.76412100	2.32754700
H	8.46774900	1.35067700	1.75718800	H	-5.47109400	-3.04103800	-0.65833800
H	7.00498000	2.03650300	2.53695100	C	-6.66630700	-3.54715300	1.00285100
N	0.60320300	-0.63287400	-1.36241800	C	-6.01802100	3.83555500	0.38365000
N	0.84101100	-0.87803000	-2.66289000	H	-4.72968100	4.15650300	-1.33556500
N	-0.30312800	-1.01221200	-3.24750700	H	-7.22433700	3.21680800	2.02821100
H	-1.15465900	-0.40592500	-0.14310600	H	-7.70502500	0.89090600	2.56423600
C	-2.74141200	-0.96080400	-2.68766900	C	-7.44547300	-3.09666300	2.10502900
H	-2.97855900	-1.99002700	-2.99998000	H	-8.17289900	-1.40086300	3.16938300
H	-2.97196100	-0.30600500	-3.54229500	H	-6.53803800	-4.61293700	0.84137800
C	-4.88894500	-0.70713100	-1.76425300	H	-6.12045200	4.89496700	0.59666200
H	-5.18511300	-0.06293700	-2.60483900	H	-7.91313600	-3.82049300	2.76478300
H	-5.14279600	-1.73094000	-2.05952900	C	3.37430000	2.85767100	-0.07077400
O	-3.49185600	-0.59888900	-1.55213300	H	4.25911500	3.20582200	0.46607900
C	-5.62541900	-0.29155100	-0.51768600	H	3.51976800	3.03784500	-1.13941200
C	-5.73105100	1.08211500	-0.22546100	O	2.21853100	3.55716200	0.38832700
C	-6.20852800	-1.24478000	0.33825800	C	2.26978600	4.89943500	0.25907000
C	-5.09035900	2.09001000	-1.01563000	O	3.22711900	5.47753800	-0.19072600
C	-6.50115000	1.51422700	0.90291200	C	0.99685800	5.53651700	0.74132500
C	-6.97668600	-0.80003400	1.46855100	H	0.15435700	5.18093400	0.14199600
C	-6.07567000	-2.66063300	0.15552100	H	0.80367600	5.25355200	1.77935200
C	-5.23041700	3.41273100	-0.72338500	H	1.08058300	6.61916400	0.65835400

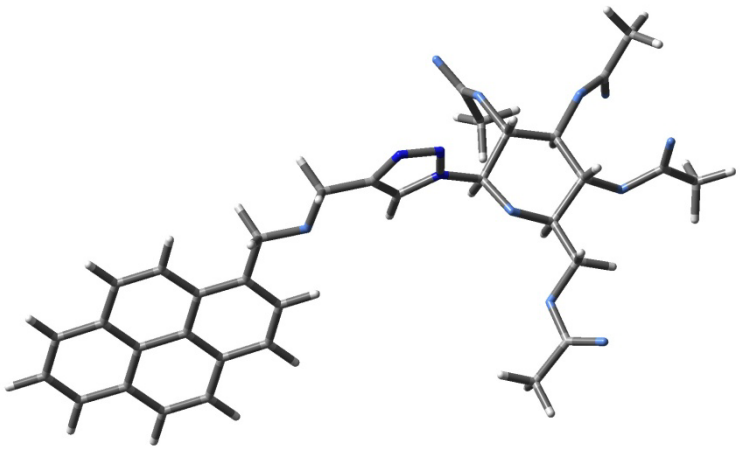


Figure S19. Calculated (cam-B3LYP/6–31G*/LANL2DZecp) structure of **6**.

Cartesian coordinates for the calculated structure of **6**.

C	3.78978700	-1.42774900	-0.33142800	N	1.76278400	-1.48594000	-2.35453800
C	5.00508600	-0.81591100	0.36131100	N	0.62275400	-1.78392400	-2.88377600
C	5.28327500	0.60794500	-0.12382400	H	-0.23602200	-0.55225800	0.02747900
C	3.99165500	1.43033700	-0.11816300	C	-1.81142100	-1.71354100	-2.32748500
C	2.59694200	-0.46223500	-0.33315500	H	-2.03659600	-2.78867300	-2.24636000
H	4.89281600	-0.76935700	1.44261600	H	-2.02417800	-1.41629400	-3.36491400
H	4.04679300	-1.58000300	-1.38134400	C	-3.96983600	-1.23994100	-1.54614400
H	3.64998000	1.54741100	0.92210000	H	-4.28853700	-1.05054900	-2.58459600
H	2.19313200	-0.30928000	0.67596400	H	-4.16463400	-2.30573200	-1.34546900
H	5.73509400	0.58498900	-1.11870700	O	-2.59317200	-0.97898300	-1.41579600
O	3.00100300	0.76667800	-0.88306500	C	4.18978900	2.79946400	-0.72427700
C	0.18682800	-0.93448100	-0.88697400	H	5.05827000	3.29272200	-0.28295100
C	-0.37537900	-1.46337900	-2.01424200	H	4.34465700	2.71844700	-1.80366100
O	3.45026500	-2.73478100	0.10686900	O	3.01018800	3.55630900	-0.45748600
C	3.12464700	-3.16905800	1.35838200	C	3.02769000	4.82601800	-0.91543900
O	2.76002700	-4.30693900	1.46311700	O	3.97714200	5.30288400	-1.48454300
C	3.27947900	-2.26884300	2.56355100	C	1.72915300	5.52357700	-0.62265600
H	4.33419100	-2.21446200	2.85192200	H	0.91366100	5.02234600	-1.15136500
H	2.91651600	-1.25159600	2.40904400	H	1.50665200	5.47592600	0.44636000
H	2.72199000	-2.72829300	3.37898400	H	1.79566700	6.56136500	-0.94602400
O	6.10725900	-1.66608500	0.05037800	C	-4.75988800	-0.37484000	-0.59467200
C	6.98193500	-1.96124100	1.03725800	C	-6.15259000	-0.53961700	-0.48273800
O	6.84538500	-1.58753200	2.17895500	C	-4.11900200	0.59344000	0.16861400
O	6.16673000	1.25242600	0.79867000	C	-6.88076100	0.28266000	0.41781300
C	7.50443800	1.16608900	0.58147200	C	-6.88297500	-1.51473300	-1.25129700
O	7.98556400	0.63060500	-0.38396600	C	-4.82694000	1.39861700	1.04917500
C	8.12839400	-2.76337700	0.50294800	H	-3.04805000	0.71193900	0.06194800
H	8.71867200	-3.15532300	1.33012600	C	-8.29457200	0.13063600	0.54914200
H	7.76658800	-3.57456100	-0.13202000	C	-6.20637200	1.26188500	1.19356200
H	8.74553200	-2.10301400	-0.11411500	C	-8.22228500	-1.65651000	-1.12713000
C	8.26078200	1.78312300	1.72001600	H	-6.34708000	-2.14994300	-1.94829700
H	8.20638100	1.09992400	2.57356700	H	-4.30409300	2.14845700	1.63640200
H	9.30190800	1.92330100	1.43220500	C	-8.98185600	-0.84127400	-0.22190400
H	7.81259100	2.73241900	2.01950500	C	-9.02036500	0.95198200	1.45218600
N	1.51994800	-0.97235500	-1.13643300	C	-6.96767700	2.07966100	2.09940500

H	-8.75124900	-2.39912400	-1.71785900	C	-11.06722200	-0.17012700	0.80546200
C	-10.36572900	-0.97584500	-0.07973000	H	-10.88835800	-1.72144900	-0.67218000
C	-10.40213400	0.78454500	1.56417900	H	-10.95586500	1.41339000	2.25561100
C	-8.30472500	1.93290100	2.22358600	H	-8.86814700	2.55678800	2.91159000
H	-6.43686800	2.82424400	2.68602300	H	-12.14186100	-0.28594800	0.90577500

Cartesian coordinates for the calculated structure of **5.**$Hg(ClO_4)_2$.

C	-3.63035100	0.65938500	0.33431200	C	-9.28273700	-0.90933200	0.82351100
C	-5.11034900	0.46593800	0.67019500	H	-9.22879200	-0.38940600	1.78541900
C	-5.74215200	-0.64597100	-0.17726900	H	-10.21221200	-0.64584500	0.32004300
C	-4.85576900	-1.89501000	-0.21895100	H	-9.23681400	-1.98288500	1.01533100
C	-2.93060400	-0.70451700	0.36273000	N	-1.52262200	-0.60030100	0.02386900
H	-5.24490300	0.23425700	1.72878600	N	-1.05020800	0.43674600	-0.65374200
H	-3.54711500	1.04538300	-0.68236200	N	0.21811200	0.22499400	-0.80571400
H	-4.84172600	-2.35583200	0.77938000	H	-0.72932700	-2.40170200	0.86331200
H	-2.98697100	-1.15155400	1.35787600	C	2.01701900	-1.39030900	-0.26925200
H	-5.92615200	-0.26392000	-1.18522600	H	2.27511900	-1.79935600	-1.25446200
O	-3.53398200	-1.52942700	-0.59633700	H	2.20181300	-2.15592200	0.48920100
C	-0.54244000	-1.49435700	0.31156400	C	4.22708100	-0.47036000	0.14716200
C	0.58865000	-0.95202400	-0.23227600	H	4.62695000	-0.79404200	-0.81115400
O	-3.03608800	1.67405100	1.13375900	H	4.63293100	0.52113600	0.35162500
C	-2.78922700	1.45375200	2.44524600	O	2.80316800	-0.23270100	-0.00778800
O	-3.01379700	0.39816900	2.99133400	C	-5.35453400	-2.90492600	-1.22413300
C	-2.20111900	2.67545100	3.08332400	H	-6.42043600	-3.09179400	-1.07893800
H	-1.29808500	2.98311900	2.54805500	H	-5.20146000	-2.53844900	-2.24318900
H	-2.91287400	3.50309500	3.01749200	O	-4.61530200	-4.10827900	-1.02334700
H	-1.97341800	2.46390200	4.12712500	C	-4.99105000	-5.14634600	-1.80195300
O	-5.73022400	1.71528300	0.37326300	O	-5.89173100	-5.07145900	-2.59895100
C	-6.75590300	2.12143700	1.15832100	C	-4.14242200	-6.35830700	-1.53610400
O	-7.14488100	1.49764300	2.11510500	H	-3.10367500	-6.14956200	-1.80737700
O	-6.97435400	-1.06277500	0.41038100	H	-4.16178000	-6.60859000	-0.47230700
C	-8.11747700	-0.45565200	-0.00224300	H	-4.51440800	-7.19545200	-2.12511900
O	-8.14776000	0.35864400	-0.88993200	Hg	2.00297900	1.69727900	-1.36228100
C	-7.34138700	3.39984400	0.63912700	Cl	3.71494300	0.47613300	-3.55065900
H	-7.97902100	3.84638700	1.40127800	O	4.04465300	0.95260300	-4.88178900
H	-6.55670400	4.09445000	0.33358200	O	2.21436600	0.33150100	-3.38287500
H	-7.94215900	3.15835300	-0.24354900	O	4.36681500	-0.79517600	-3.22332800

O	4.09310800	1.52197900	-2.50560400
Cl	1.61135200	4.11432400	0.40999300
O	2.32550800	5.37836400	0.37253700
O	1.02331600	3.80613700	-0.96858300
O	2.57039500	2.96251900	0.64969200
O	0.54747300	4.09176100	1.41019000
C	4.53523900	-1.42328300	1.26947000
C	5.05180000	-2.70894900	1.00514900
C	4.30579100	-0.99986600	2.59611900
C	5.28314900	-3.22076000	-0.31617500
C	5.36881200	-3.57588400	2.10763200
C	4.62978500	-1.87564100	3.68380400
C	3.75765100	0.28428200	2.91859900
C	5.78289600	-4.47234300	-0.51408200
H	5.06015100	-2.61313000	-1.18474400
C	5.89655800	-4.88001600	1.85361600
C	5.15442700	-3.13632000	3.40994100
C	4.41118500	-1.44190100	5.02715200
H	3.47277200	0.96816200	2.12866700
C	3.56584500	0.66139400	4.21424200
C	6.09915000	-5.32027700	0.58397400
H	5.94613800	-4.82847300	-1.52635900
H	6.13100500	-5.51122200	2.70610200
H	5.40131500	-3.79711100	4.23731000
C	3.89670900	-0.21022100	5.28870900
H	4.66826600	-2.12155400	5.83466100
H	3.15236600	1.64157000	4.42941300
H	6.50071200	-6.31157900	0.40039900
H	3.73537900	0.11322100	6.31204000

Cartesian coordinates for the calculated structure of **5.**$Pb(ClO_4)_2$.

C	3.55232500	-0.79646800	0.09191300	C	-2.09536500	1.13444400	0.51278500
C	5.02826200	-0.81660400	0.49036400	H	-2.38162600	2.10360400	0.09301200
C	5.70654500	0.52792900	0.19589800	H	-2.34953200	1.11065200	1.57385300
C	4.85428800	1.70819800	0.67542200	C	-4.22609500	-0.03844600	0.12057400
C	2.88869400	0.45008600	0.68778500	H	-4.74730900	0.69292000	-0.49045600
H	5.14600000	-1.05735800	1.54882500	H	-4.46760900	-1.03337500	-0.25464600
H	3.47998700	-0.71317800	-0.99321700	O	-2.79146400	0.08328900	-0.16818500
H	4.83238500	1.70753400	1.77488800	C	5.40240200	3.02949400	0.19250900
H	2.93402900	0.43307900	1.77875200	H	6.46986500	3.10172000	0.41029900
H	5.90376500	0.59937200	-0.87729600	H	5.25995400	3.13101100	-0.88718700
O	3.53066100	1.58173700	0.17030200	O	4.69297000	4.06076700	0.87582400
C	0.46694800	1.01039300	1.09209200	C	5.11802900	5.31631400	0.61617300
C	-0.64489100	0.85602300	0.31183600	O	6.03986300	5.55314000	-0.12312700
O	2.90126800	-2.02702100	0.38285200	C	4.29186000	6.33156400	1.35509300
C	2.63320800	-2.36991300	1.66385000	H	3.26096400	6.30408300	0.99068300
O	2.88804100	-1.65446600	2.60561000	H	4.27045400	6.09926700	2.42282900
C	1.97268300	-3.71288600	1.72546500	H	4.71095800	7.32390500	1.19456100
H	1.01035300	-3.67716300	1.20457700	Cl	-3.44945500	2.27681500	-2.81275000
H	2.59115300	-4.45666600	1.21664400	O	-3.56029200	3.02249100	-4.05395800
H	1.82471100	-3.99425500	2.76720900	O	-1.99123500	1.96577500	-2.51174500
O	5.62090400	-1.84458900	-0.30098800	O	-4.01897100	3.00018900	-1.67149600
C	6.61954200	-2.57608500	0.24683500	O	-4.09318900	0.92185400	-2.93366400
O	7.00556300	-2.42689100	1.38023400	Cl	-1.50868400	-3.47969200	-1.18413900
O	6.93562000	0.61803000	0.91642300	O	-1.68848900	-4.71948000	-1.92128400
C	8.07203400	0.20494700	0.29803900	O	-0.44884200	-2.62041000	-1.81127400
O	8.10298200	-0.15930100	-0.85027700	O	-2.76973200	-2.63018200	-1.28256300
C	7.18287700	-3.53441100	-0.75881800	O	-1.19443100	-3.71129900	0.22794700
H	7.78791000	-4.28436400	-0.25049300	Pb	-1.94237500	-0.52904000	-2.37960400
H	6.38778800	-4.00527400	-1.33984400	C	-4.56987000	0.08248900	1.58038000
H	7.81341600	-2.96335900	-1.44781100	C	-5.24216000	1.22585000	2.06628900
C	9.22887200	0.23004800	1.25031900	C	-4.24188800	-0.97870800	2.45224500
H	9.13787500	-0.64288800	1.90468200	C	-5.56026900	2.36913100	1.25995900
H	10.16278400	0.17012200	0.69261200	C	-5.63240500	1.27224600	3.44957600
H	9.20712800	1.12527900	1.87448300	C	-4.62971900	-0.91141000	3.83087000
N	1.48390500	0.52652900	0.33315400	C	-3.52097100	-2.13699200	2.02239500
N	1.05181200	0.09085400	-0.84042400	C	-6.21732400	3.44283400	1.78149800
N	-0.22787500	0.29110300	-0.85061300	H	-5.26137000	2.40813200	0.22051200
H	0.61889400	1.39380000	2.08825200	C	-6.32873300	2.41508700	3.95184800

C	-5.32229000	0.20623700	4.28800700	H	-5.62457900	0.25085000	5.33154900
C	-4.30153100	-1.98994400	4.70798600	C	-3.61724600	-3.07533100	4.25510500
H	-3.19088900	-2.22004300	0.99640800	H	-4.61156200	-1.91929500	5.74680000
C	-3.22031700	-3.14332000	2.89107500	H	-2.66576500	-4.00273800	2.52883500
C	-6.61755700	3.47073300	3.14610900	H	-7.14579800	4.33502000	3.53560900
H	-6.43628900	4.29330300	1.14360300	H	-3.37076000	-3.89012300	4.92851800
H	-6.61848200	2.41703500	4.99885200				

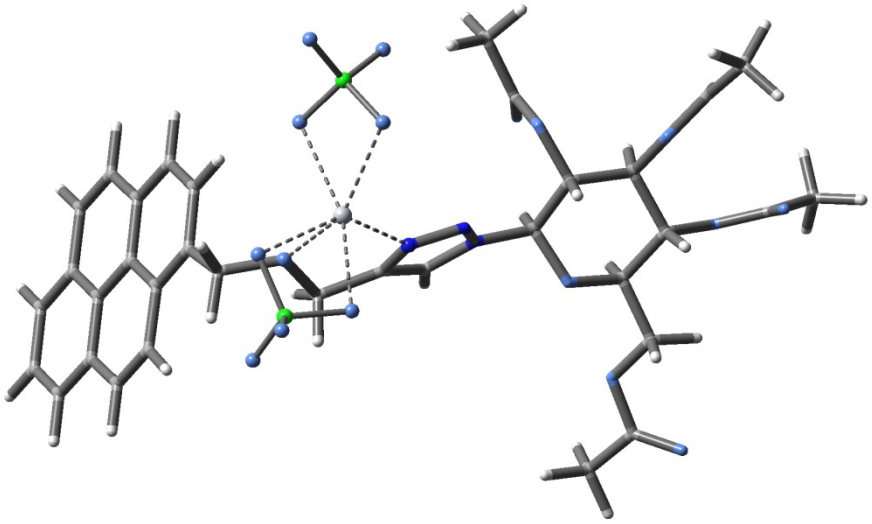


Figure S20. Calculated (cam-B3LYP/6–31G*/LANL2DZecp) structure for **6.**$Hg(ClO_4)_2$.

Cartesian coordinates for the calculated structure of **6.Hg(ClO$_4$)$_2$**.

C	-3.92560200	-0.06395000	-0.68407300	C	1.83005500	0.58446400	1.04836500
C	-5.32477400	0.48761400	-0.96735300	H	1.97419100	0.72533800	2.12817700
C	-5.87309800	1.29341700	0.21728300	H	2.24053800	1.45502500	0.52606200
C	-4.82436800	2.26470700	0.76660600	C	3.93611900	-0.51692000	0.67628900
C	-3.03761300	1.05909900	-0.13672300	H	4.23473300	-0.23409100	1.68655500
H	-5.32417800	1.11677300	-1.85959700	H	4.26371400	-1.54514800	0.51926400
H	-4.00017200	-0.82736300	0.09123900	O	2.49378200	-0.59667200	0.63388600
H	-4.63437800	3.04709400	0.01767300	C	-5.27353400	2.91128700	2.05462800
H	-2.90718100	1.85043600	-0.87850600	H	-6.27960100	3.32063400	1.94416300
H	-6.21016000	0.60254400	0.99496600	H	-5.28297300	2.17966200	2.86761300
O	-3.62009100	1.55705500	1.03649000	O	-4.35028300	3.95759400	2.35200700
C	-0.58859800	1.32759600	0.36667900	C	-4.66253700	4.70545500	3.43289200
C	0.37784000	0.42819500	0.72438200	O	-5.65069000	4.51409300	4.09536200
O	-3.39988700	-0.76462800	-1.80466000	C	-3.62595800	5.76691800	3.67503800
C	-3.02159300	-0.08812800	-2.91429200	H	-2.66332400	5.30003600	3.90186100
O	-3.05515500	1.11833700	-2.99462600	H	-3.49325200	6.37793900	2.77849100
C	-2.55961700	-1.03532000	-3.97871600	H	-3.93734500	6.39140400	4.51120500
H	-1.75014200	-1.66433600	-3.59758300	C	4.45430100	0.39506100	-0.40572300
H	-3.38074800	-1.70060400	-4.25992200	C	5.20487900	1.55800600	-0.14947300
H	-2.22694400	-0.46836400	-4.84706200	C	4.14095100	0.04671000	-1.72197200
O	-6.14015500	-0.66023900	-1.19367100	C	5.63162800	2.35880000	-1.25059500
C	-7.12945500	-0.56977800	-2.11378600	C	5.57596600	1.99092300	1.17656000
O	-7.33009500	0.41916200	-2.77528200	C	4.55163600	0.82286700	-2.78970900
O	-6.96718400	2.10180800	-0.21465200	H	3.55913800	-0.85293400	-1.90427400
C	-8.22098600	1.58858400	-0.11243800	C	6.39431200	3.54653300	-1.02817300
O	-8.45656700	0.52166800	0.39562300	C	5.29918600	1.98453800	-2.57814400
C	-7.93715300	-1.83206700	-2.14394100	C	6.29762300	3.11542500	1.38167800
H	-8.54829400	-1.85385900	-3.04554500	H	5.28074500	1.39882000	2.03436200
H	-7.29247900	-2.71127000	-2.09028000	H	4.29904600	0.52944700	-3.80431700
H	-8.58700800	-1.83437000	-1.26297800	C	6.73625900	3.93952600	0.29084000
C	-9.21963600	2.50585100	-0.75017800	C	6.81632700	4.34228300	-2.12628600
H	-9.14174300	2.37676900	-1.83450200	C	5.74031700	2.80801000	-3.67080000
H	-10.22359900	2.23689200	-0.42377700	H	6.56496800	3.41408000	2.39133600
H	-9.00291000	3.54981600	-0.51652600	C	7.48316700	5.10280200	0.49026200
N	-1.71048300	0.58023200	0.21143200	C	7.56185500	5.49948100	-1.88407500
N	-1.47700100	-0.70113600	0.45271100	C	6.46234500	3.93017400	-3.45673600
N	-0.22078000	-0.79255200	0.76020100	H	5.47808600	2.50250900	-4.67949500
H	-0.57756100	2.39447600	0.21057900	C	7.89171800	5.87519200	-0.58901500

H	7.74376400	5.39729000	1.50279800	O	3.56565000	-1.95912700	3.68861400
H	7.88375200	6.10537000	-2.72620100	O	3.17227500	-3.51512700	1.85062500
H	6.79105800	4.54371500	-4.29058300	Cl	0.77501800	-3.89049600	-2.00151300
H	8.47256400	6.77624500	-0.41952700	O	1.42056100	-5.07505500	-2.54032200
Hg	1.19556700	-2.70831000	0.75459600	O	0.09169800	-4.22671400	-0.67450200
Cl	2.79235100	-3.13069500	3.27734700	O	1.80440800	-2.84571400	-1.61501300
O	2.96113100	-4.26591800	4.16675700	O	-0.20258700	-3.31080700	-2.91861100
O	1.32233300	-2.75482000	3.16337500				

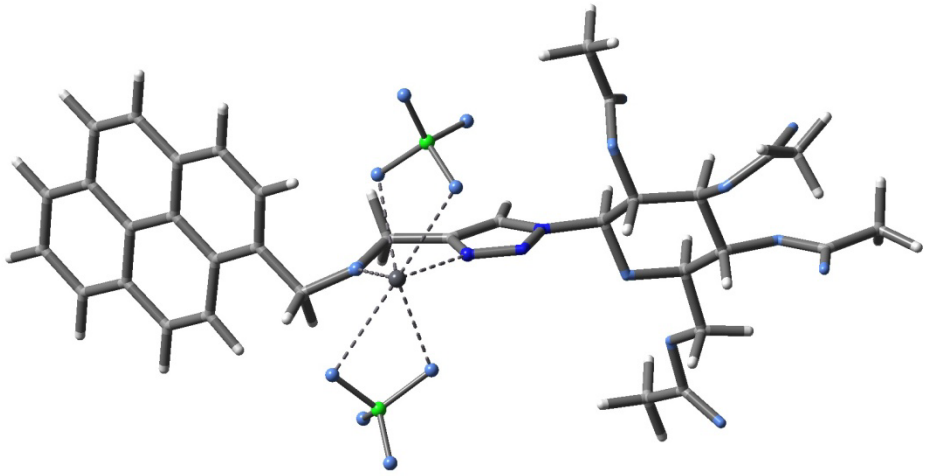


Figure S21. Calculated (cam-B3LYP/6–31G*/LANL2DZecp) structure for **6.**$Pb(ClO_4)_2$.

Cartesian coordinates for the calculated structure of **6.**$Pb(ClO_4)_2$.

C	-4.19107800	-0.74606800	-0.65328700	C	-0.80240400	0.61885800	-1.35335600
C	-5.64706500	-0.44074400	-1.01226000	C	0.23338000	0.26643500	-0.53279300
C	-6.06560400	0.96231900	-0.55808700	O	-3.78638200	-2.02210800	-1.13509700
C	-5.00956100	2.00609900	-0.93269200	C	-3.64186900	-2.22879800	-2.46461000
C	-3.29614000	0.42043200	-1.08545900	O	-3.76898600	-1.35033000	-3.28700600
H	-5.81320100	-0.53301100	-2.08705100	C	-3.29202900	-3.65702000	-2.74735200
H	-4.10753100	-0.83507600	0.43063400	H	-2.30233400	-3.86575100	-2.33129300
H	-4.97733400	2.10600000	-2.02734500	H	-4.00649600	-4.32382700	-2.25879900
H	-3.29796200	0.53095600	-2.17191700	H	-3.29161500	-3.82187700	-3.82398700
H	-6.24062000	0.95429800	0.52120300	O	-6.41708100	-1.42608400	-0.32477300
O	-3.73922900	1.58761300	-0.45089900	C	-7.53181200	-1.90080600	-0.92748700

O	-7.88495500	-1.56311200	-2.03082400
O	-7.25999100	1.35274100	-1.23616600
C	-8.45078900	1.08570900	-0.64114000
O	-8.54537300	0.60675100	0.46068100
C	-8.26029600	-2.84418100	-0.01811400
H	-8.99440300	-3.41046000	-0.59025300
H	-7.56443100	-3.51350900	0.49110000
H	-8.77278100	-2.24624100	0.74224400
C	-9.58597700	1.42563100	-1.55868900
H	-9.65690600	0.62887300	-2.30609700
H	-10.51389600	1.47396500	-0.98995400
H	-9.40285900	2.36595500	-2.08187700
N	-1.91418300	0.21402400	-0.68950800
N	-1.61468000	-0.34577000	0.46837500
N	-0.32115800	-0.31836200	0.55620500
H	-0.84727800	1.09869100	-2.31773700
C	1.71608300	0.37856500	-0.67788000
H	1.99589800	1.40124700	-0.95316100
H	2.07880300	-0.30432400	-1.45086600
C	3.64105300	0.61459200	0.74923600
H	3.53438100	1.69828300	0.66495300
H	3.89372300	0.40033100	1.78884700
O	2.32226400	0.05321400	0.57199700
C	-5.30758200	3.35374500	-0.32073600
H	-6.33968800	3.64510400	-0.52526100
H	-5.16255600	3.32190300	0.76292100
O	-4.40873800	4.29534100	-0.90369100
C	-4.60367600	5.57879000	-0.53134600
O	-5.48497600	5.91452900	0.21897100
C	-3.58612400	6.48668100	-1.16379300
H	-2.59079600	6.24846500	-0.77771900
H	-3.56467400	6.33901500	-2.24640100
H	-3.83074900	7.52177500	-0.92941300
C	4.66201200	0.05815100	-0.21398300
C	5.79301800	0.81856200	-0.57068500
C	4.50903100	-1.23206100	-0.71793700
C	6.74584800	0.26052200	-1.46892600
C	6.04691300	2.14173600	-0.05531000
C	5.43669700	-1.77543300	-1.59310500
H	3.64460700	-1.82295400	-0.43241400
C	7.89782600	1.01106600	-1.85682100
C	6.55909400	-1.04765600	-1.98781000
C	7.14128100	2.84706300	-0.42152400
H	5.35876400	2.58127500	0.65737000
H	5.28991400	-2.78050800	-1.97742100
C	8.10742600	2.31472800	-1.33971100
C	8.84211200	0.45548000	-2.76069900
C	7.53202200	-1.58556400	-2.90039800
H	7.31012200	3.84028000	-0.01540900
C	9.23953400	3.03509000	-1.73032500
C	9.95976100	1.20923000	-3.12710500
C	8.61720400	-0.87053600	-3.26985300
H	7.37133100	-2.58778500	-3.28688900
C	10.15554700	2.48624900	-2.61690200
H	9.39616300	4.03263700	-1.33008000
H	10.68034300	0.78265700	-3.81901300
H	9.34542200	-1.28709800	-3.95974900
H	11.03045500	3.05685400	-2.91192200
Cl	1.71937900	1.42884200	3.75444700
O	1.39114500	1.80298700	5.11904200
O	0.47491500	0.89881400	3.04686300
O	2.26825800	2.54000000	2.97979500
O	2.66743200	0.26034000	3.72627800
Cl	0.29317700	-3.49392900	-0.04191100
O	-0.48398000	-2.97199800	-1.17224300
O	1.53512200	-2.62422300	0.12307000
O	-0.45443300	-3.30583400	1.23954800
O	0.67951300	-4.88167200	-0.23611500
Pb	1.08372700	-1.30263200	2.20456500

Table S1. Distance of metal to donor center and Weiberg Bond Indices (WBI) of all the model complexes

	Compound	**Distances** (Å)	**WBI**	**Compound**	**Distances** (Å)	**WBI**
d_{M-N}	**3**.$Cu(ClO_4)_2$	2.05274	0.2596	**5**.$Pb(ClO_4)_2$	2.43925	0.1556
d_{M-O}		1.97460	0.2674		2.44669	0.1213
$d_{M-O\ (perchlorate)}$		2.61836	0.0960		2.51054	0.1199
$d_{M-O\ (perchlorate)}$		2.008	0.2776		2.63201	0.0970
$d_{M-O\ (perchlorate)}$		1.95217	0.3183		2.49879	0.1152
$d_{M-O\ (perchlorate)}$		2.29946	0.1738		2.65294	0.0937
d_{M-N}	**4**.$Cu(ClO_4)_2$	2.05655	0.2575	**6**.$Hg(ClO_4)_2$	2.38248	0.2480
d_{M-O}		1.97404	0.3673		2.48172	0.1385
$d_{M-O\ (perchlorate)}$		2.61904	0.0959		2.41256	0.2196
$d_{M-O\ (perchlorate)}$		2.00925	0.2774		2.39992	0.2258
$d_{M-O\ (perchlorate)}$		2.29585	0.1751		2.45043	0.1945
$d_{M-O\ (perchlorate)}$		1.95093	0.3193		2.35932	0.2574
d_{M-N}	**5**.$Hg(ClO_4)_2$	2.37974	0.2477	**6**.$Pb(ClO_4)_2$	2.37899	0.1678
d_{M-O}		2.48994	0.1413		2.45715	0.1118
$d_{M-O\ (perchlorate)}$		2.44803	0.1990		2.43444	0.1335
$d_{M-O\ (perchlorate)}$		2.38884	0.2567		2.69567	0.0865
$d_{M-O\ (perchlorate)}$		2.44353	0.2333		2.50659	0.1112
$d_{M-O\ (perchlorate)}$		2.35839	0.1995		2.70370	0.0856

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