**Supporting Information**

*for*

# Synthesis and Sensing Properties of 1,1′-Disubstituted Unsymmetrical Ferrocene-Triazole Derivatives: A Multichannel Probe for Hg(II) Ion

Dipendu Mandal, Pranab Deb, Bijan Mondal, Arunabha Thakur, Joseph Ponniah S 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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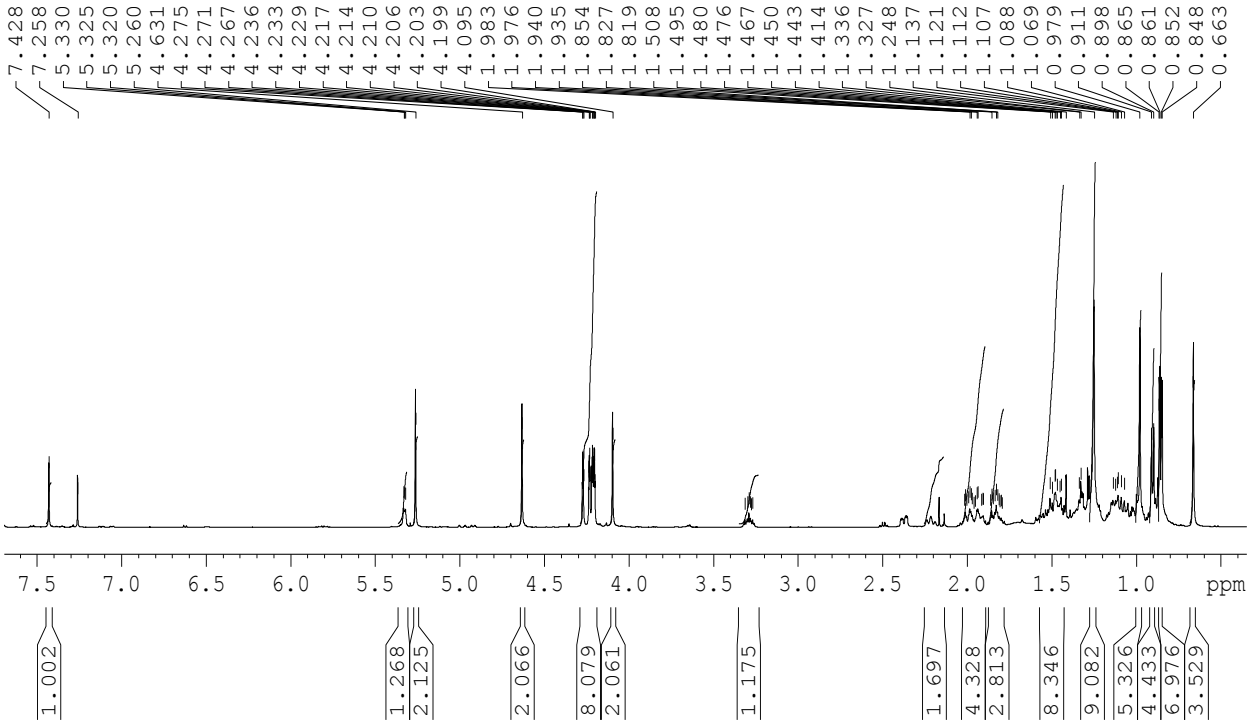
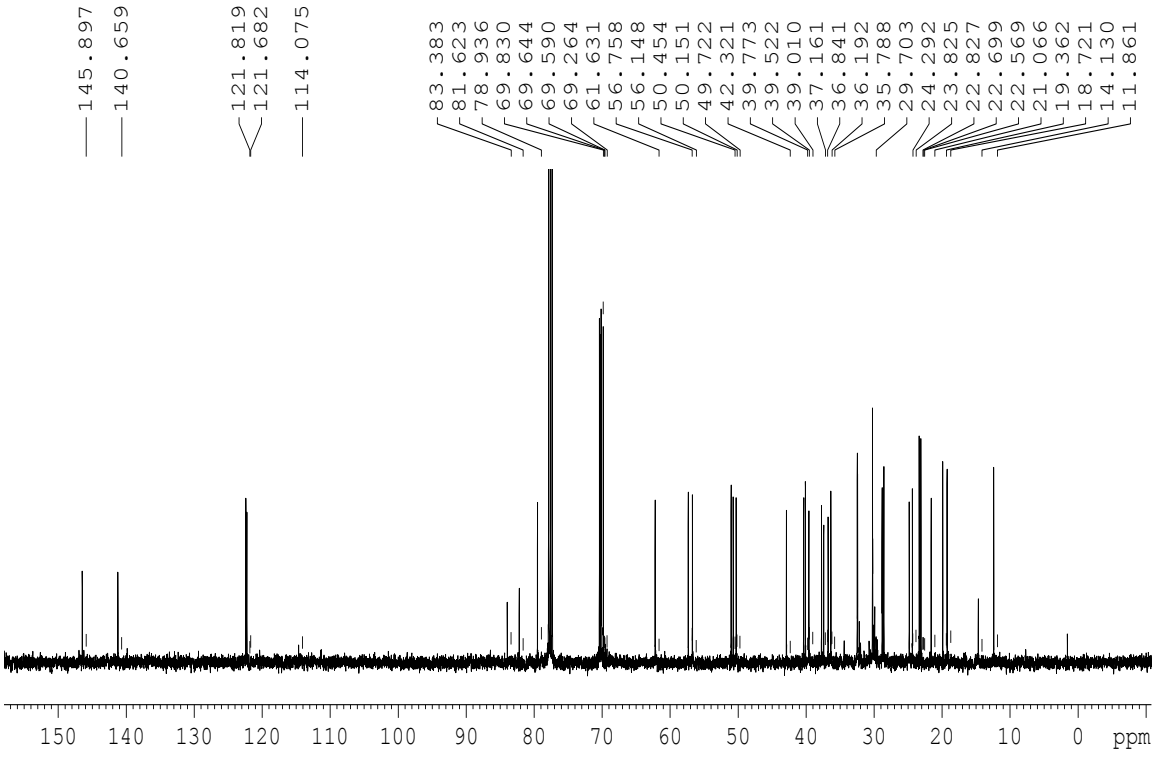
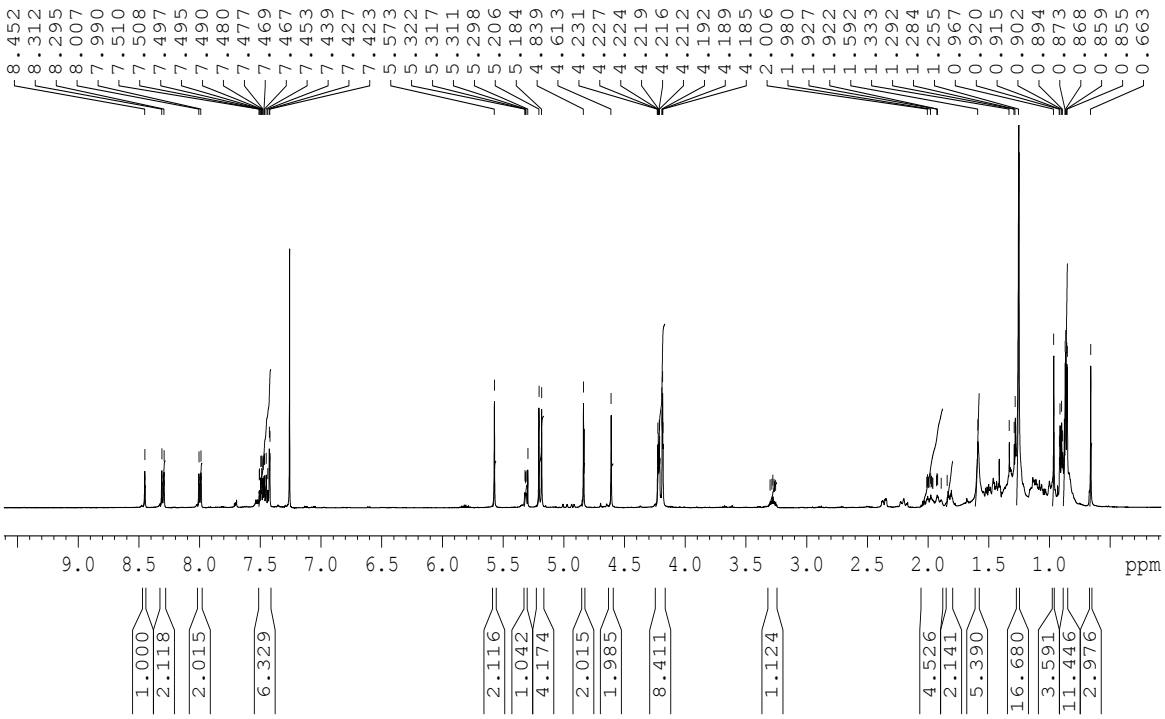


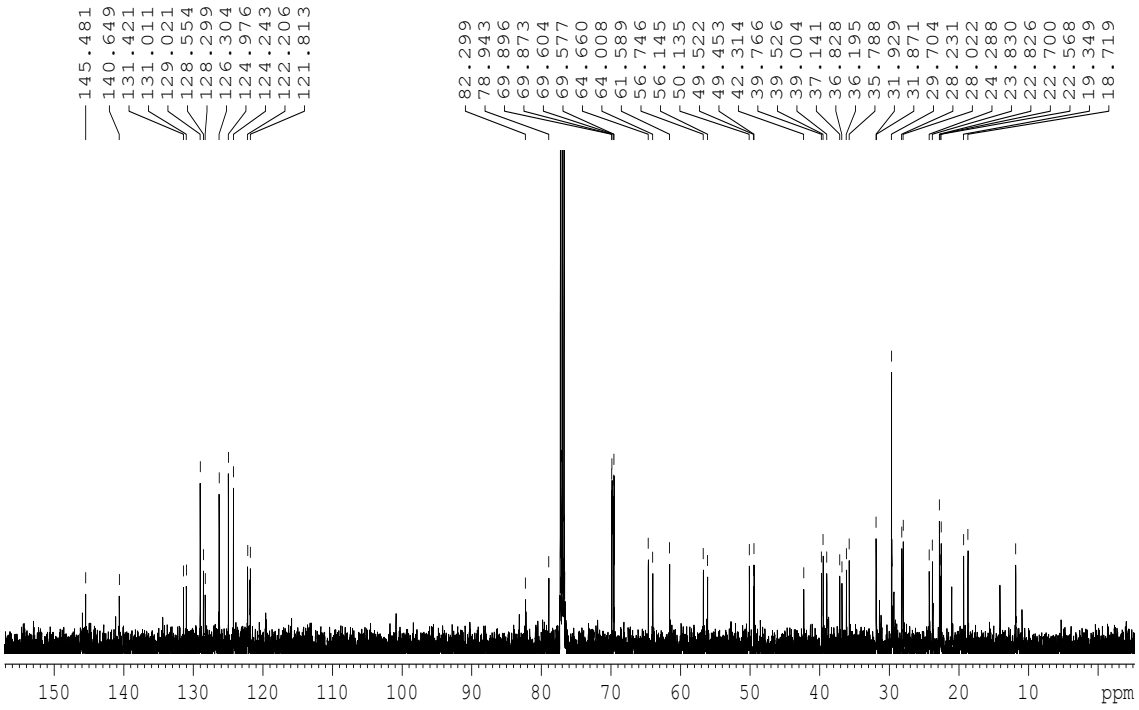

**$^{1}$H NMR spectrum of 3**



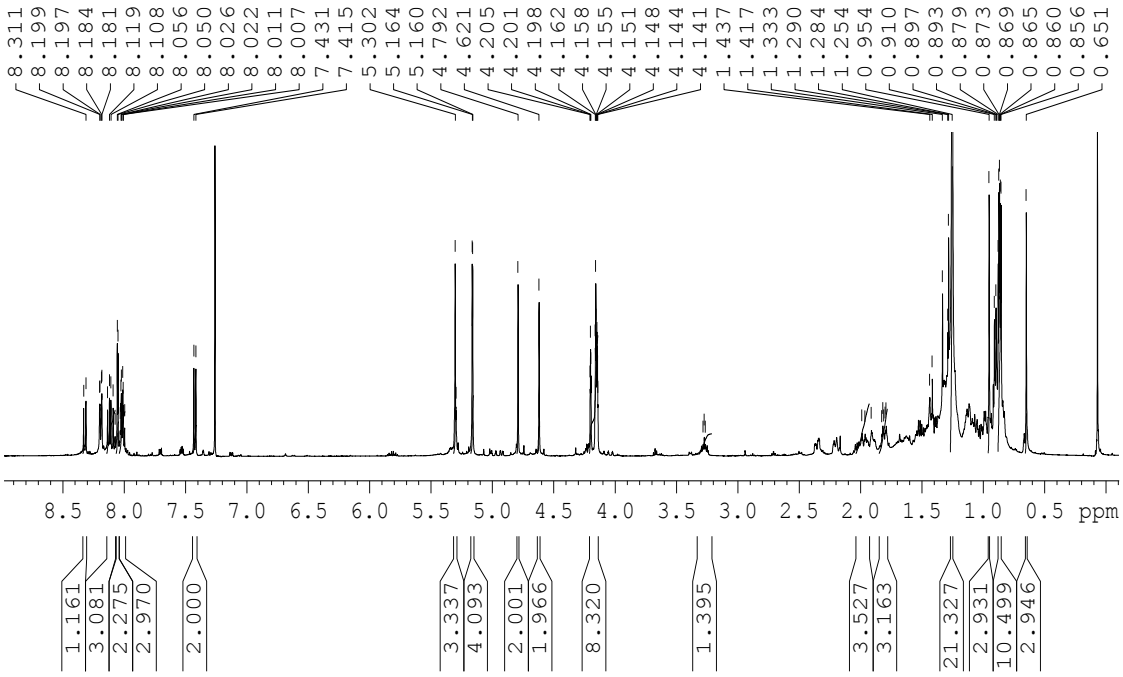

**$^{13}$C NMR spectrum of 3**



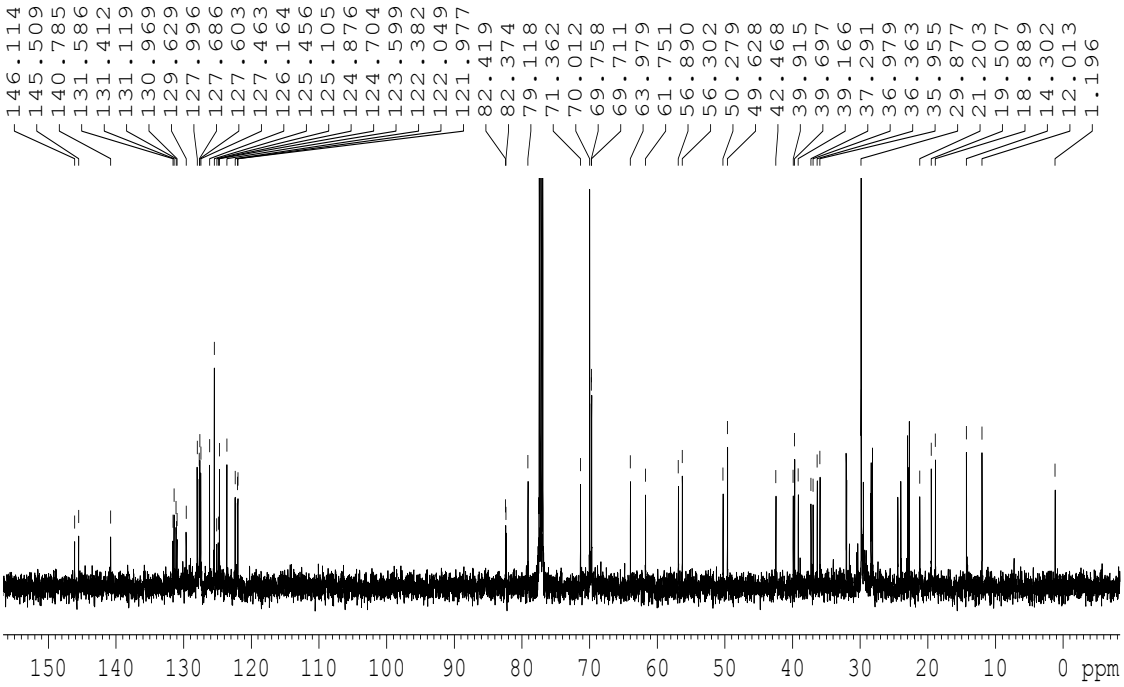

**$^{1}$H NMR spectrum of 4**



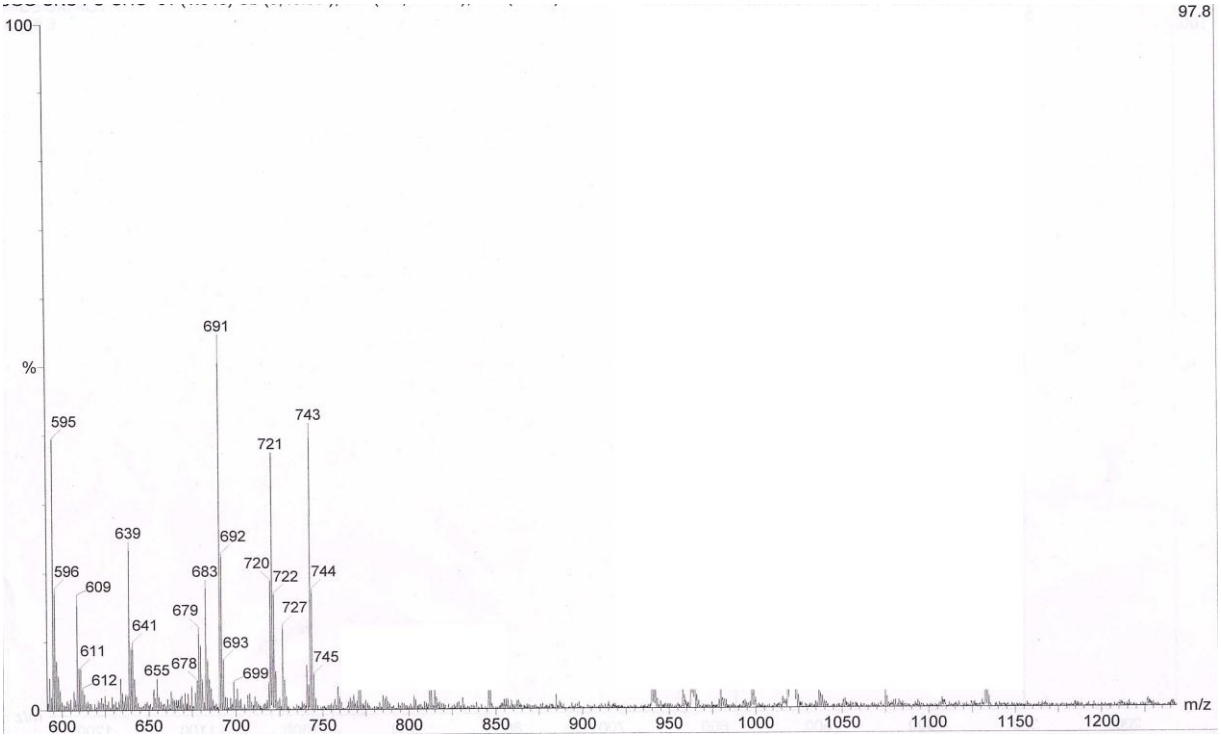

**$^{13}$C NMR spectrum of 4**



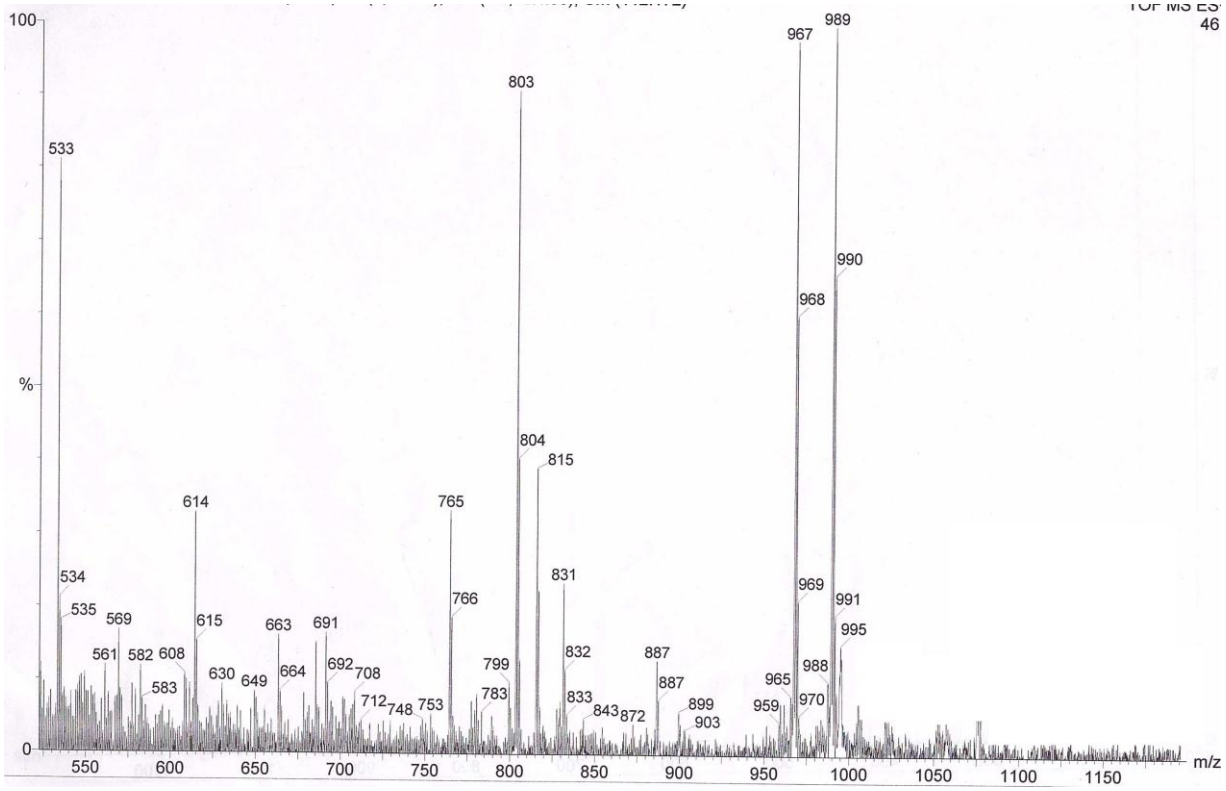

**$^{1}$H NMR spectrum of 5**



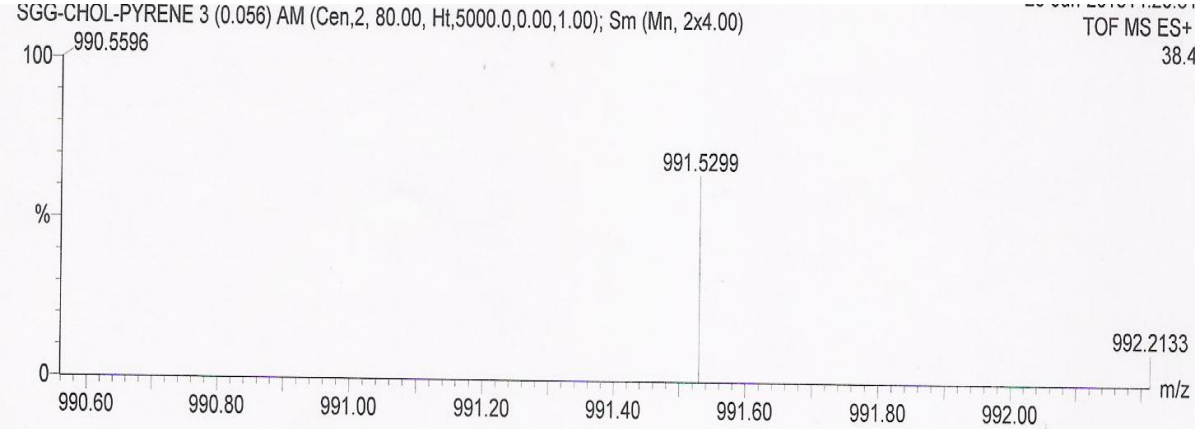

**$^{13}$C NMR spectrum of 5**




Electospray mass spectrum of **3**.




Electospray mass spectrum of **4**.




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 991.5299 | 991.5301 | -0.2 | -0.2 | 28.5 | 1 | C62 H75 N6 O2 Fe |

HRMS for the compound **5**

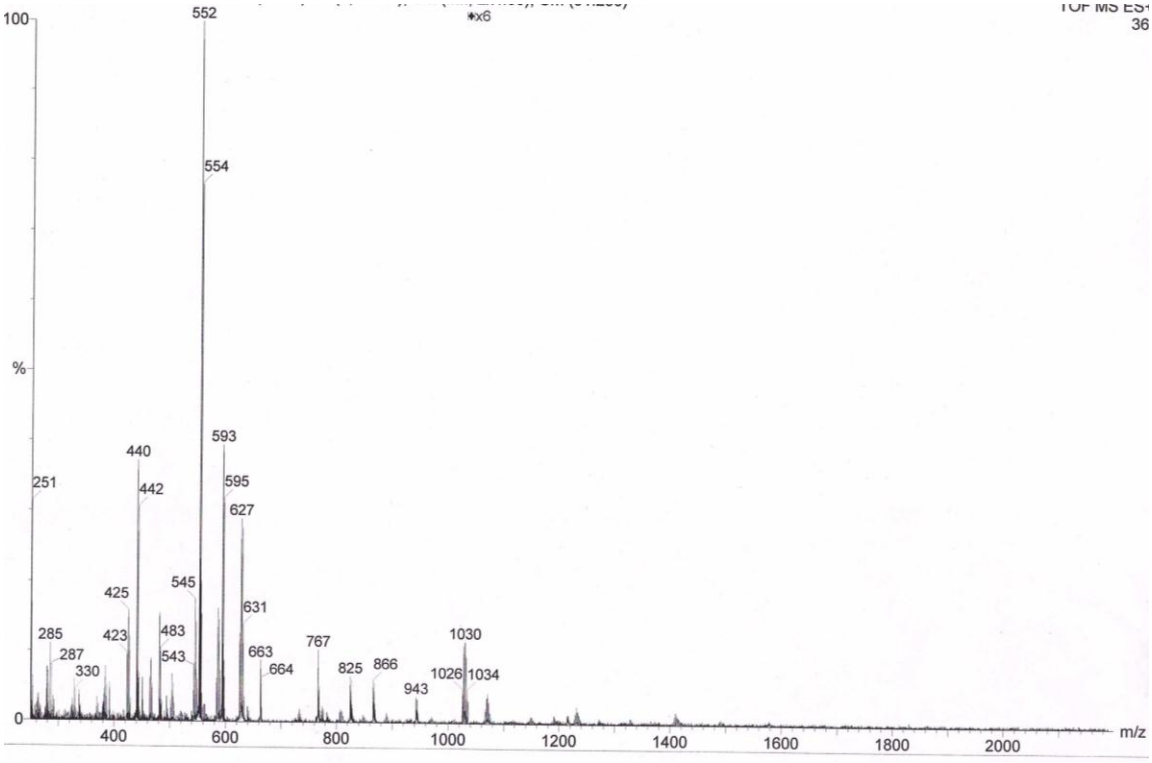



**Figure S1.** Electospray mass spectrum of [**4.Cu**$^{2+}$]

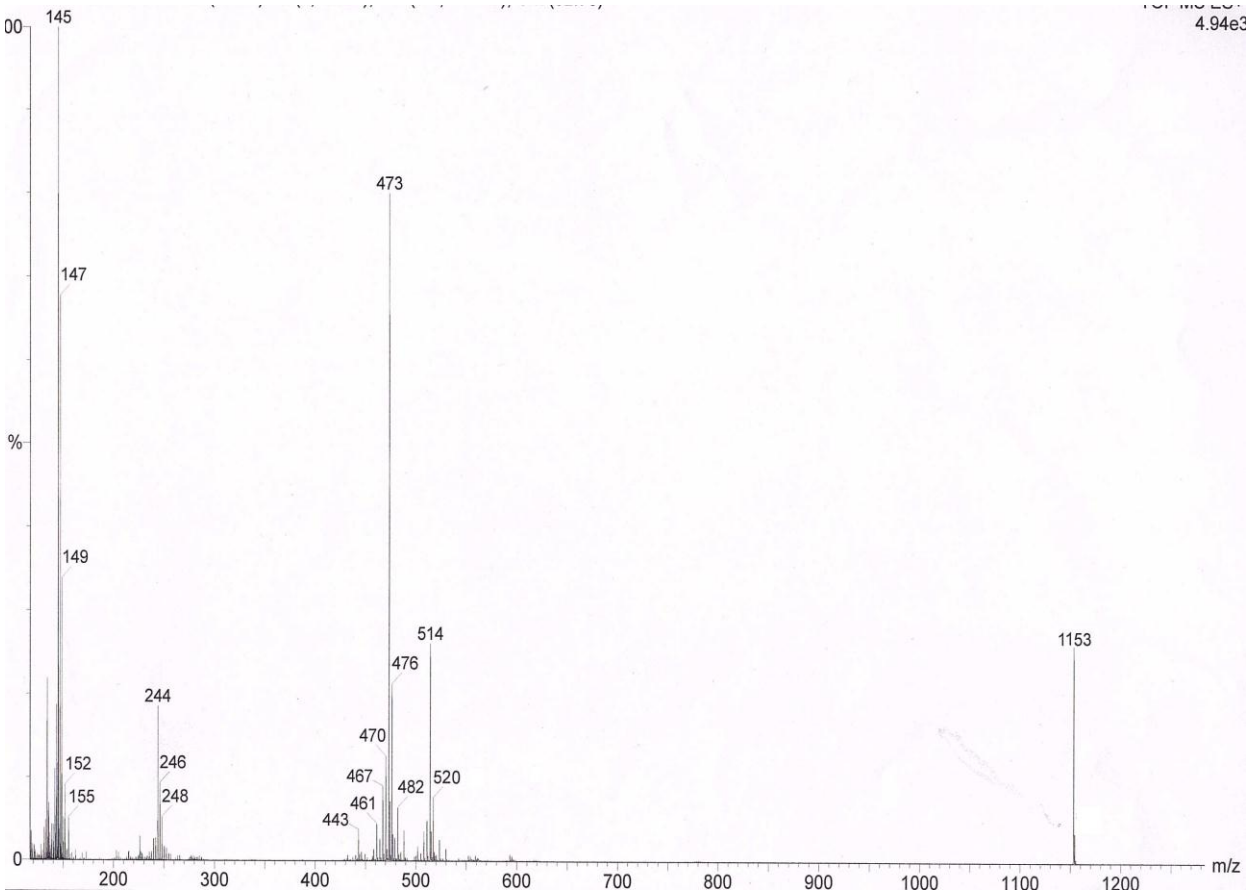



**Figure S2.** Electospray mass spectrum of [**5**.$Cu^{2+}$]

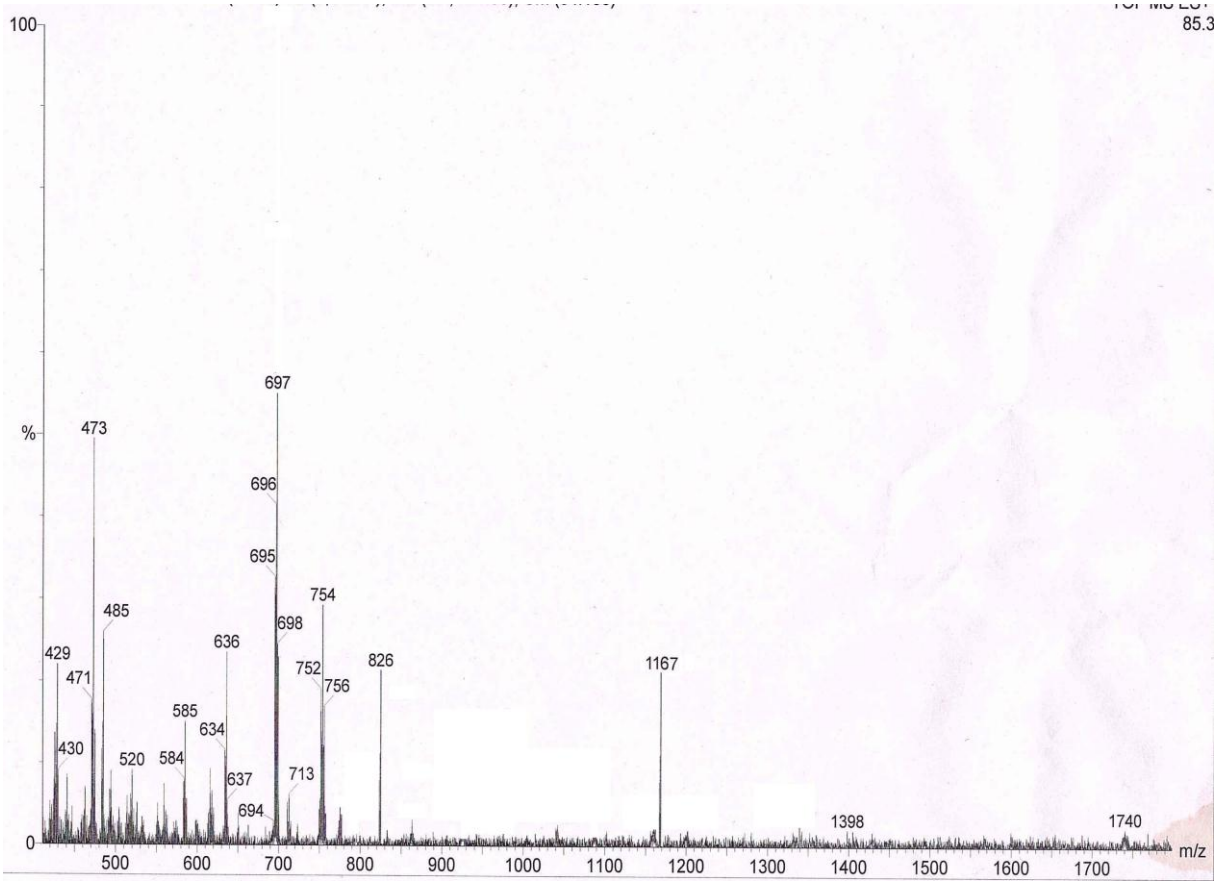



**Figure S3.** Electospray mass spectrum of [**4.Hg**$^{2+}$]

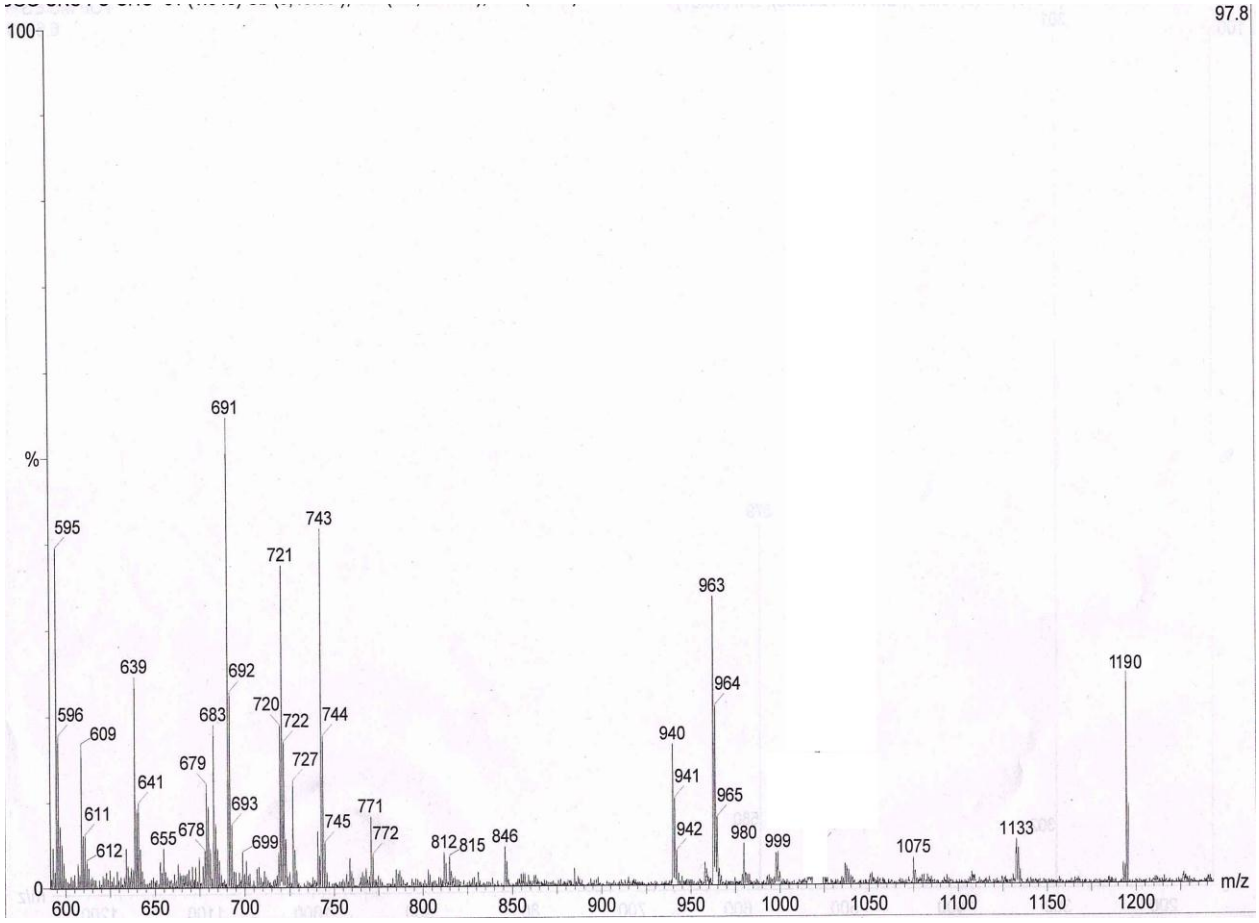



**Figure S4.** Electospray mass spectrum of [**5**.$Hg^{2+}$]

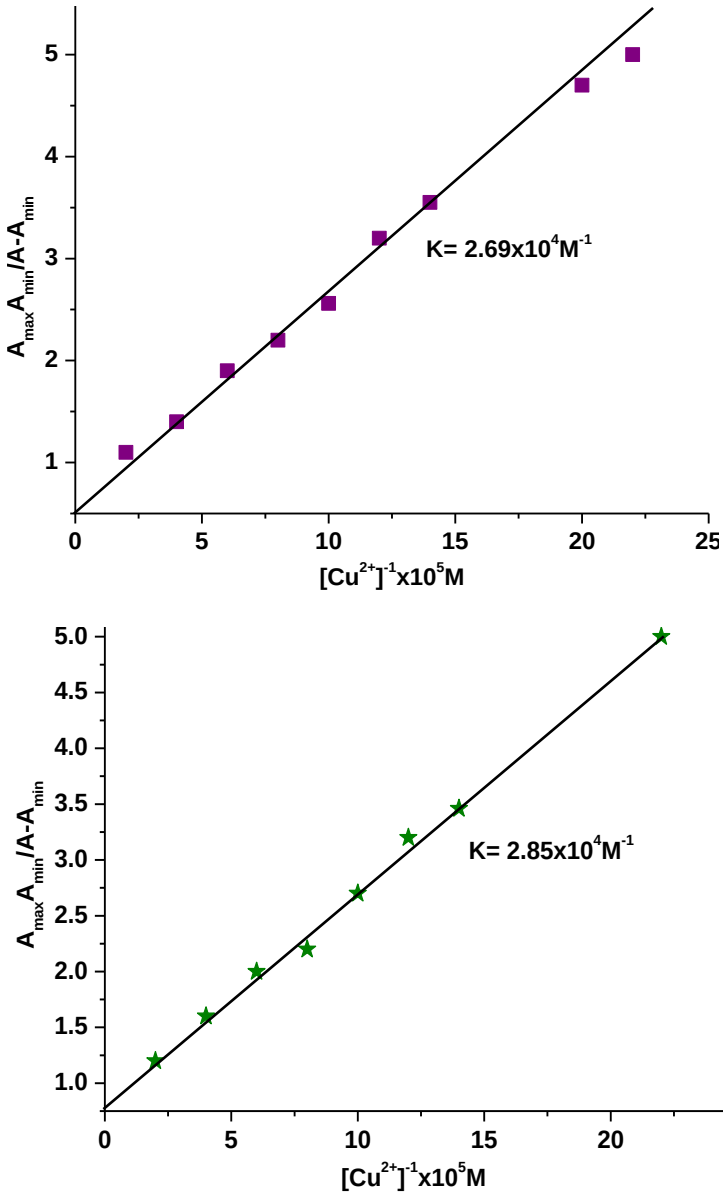



**Figure S5.** Quantitative binding data (Benesi-Hildebrand plot) for **4** (top) and **5** (bottom) with $Cu^{2+}$ ion.

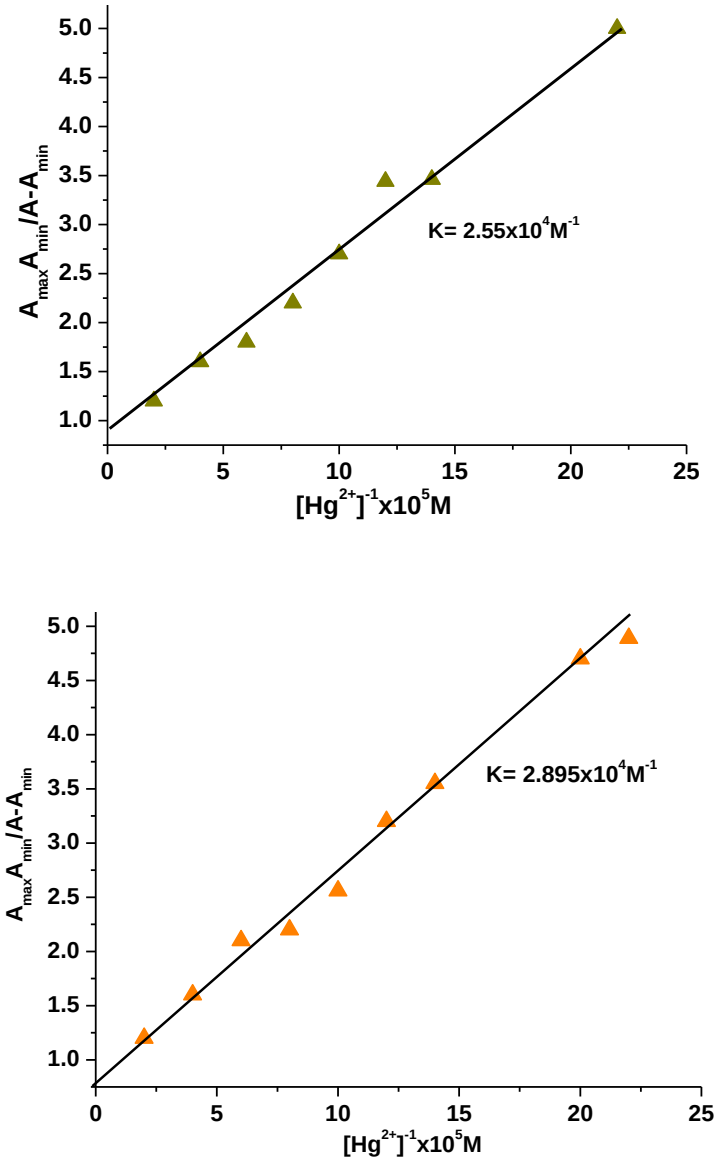



**Figure S6.** Quantitative binding data (Benesi-Hildebrand plot) for **4** (top) and **5** (bottom) with $Hg^{2+}$ion.

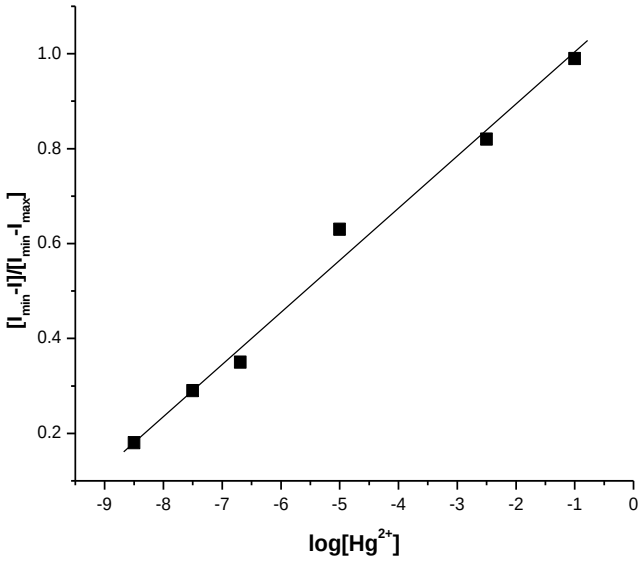



**Figure S7.** Fluorescence intensity of **4** or **5** at each concentration of 2 nM at each concentration of $Hg^{2+}$ normalized between the minimum fluorescence intensity and the maximum fluorescence intensity.

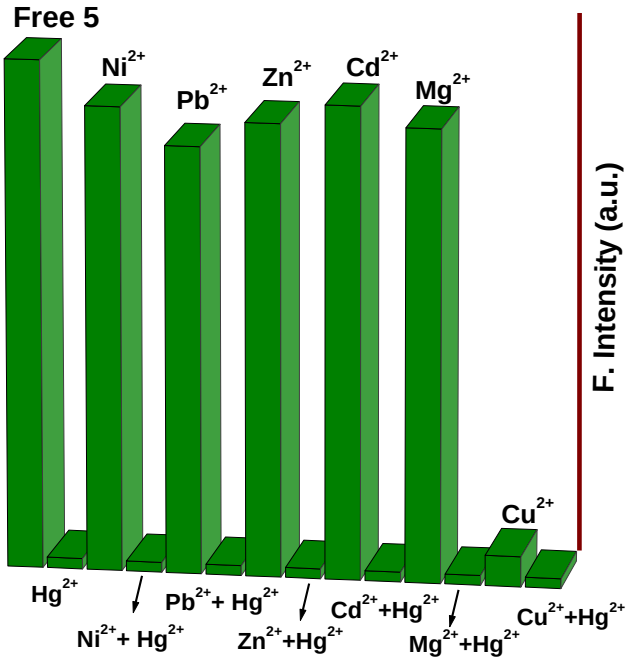



**Figure S8**. Bar plot representation of changes in fluorescence spectra of **5** ($1\times10^{-7}$ M) in $CH_3CN/H_2O$ (5:5) upon addition of the several metal cations.

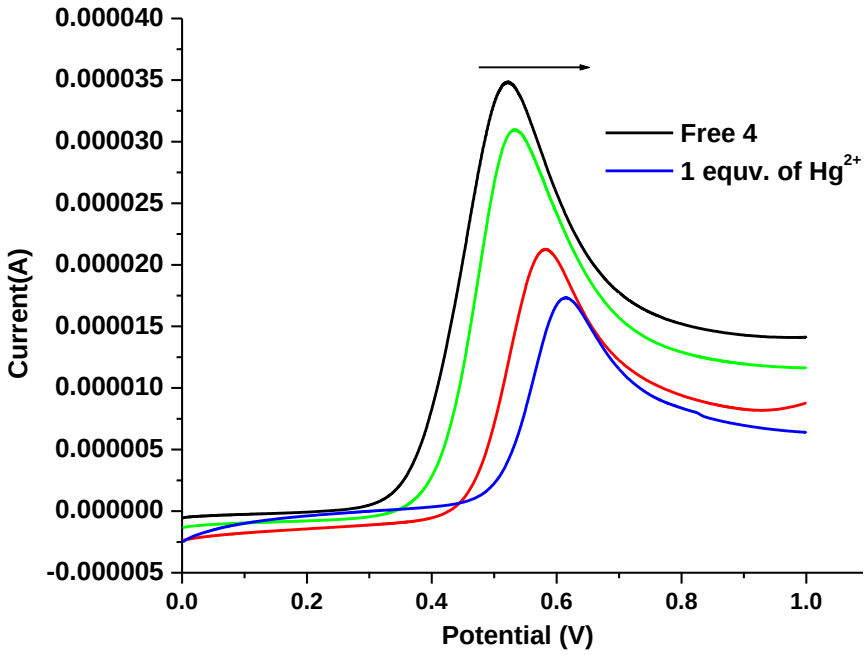



**Figure S9**. Evolution of LSV of **4** ($1x10^{-4}$ M) upon addition of $Hg^{2+}$ up to 1 equiv with [(*n*-Bu)$_4$N]$ClO_4$ as supporting electrolyte. Scan rate employed 0.1 $Vs^{-1}$.

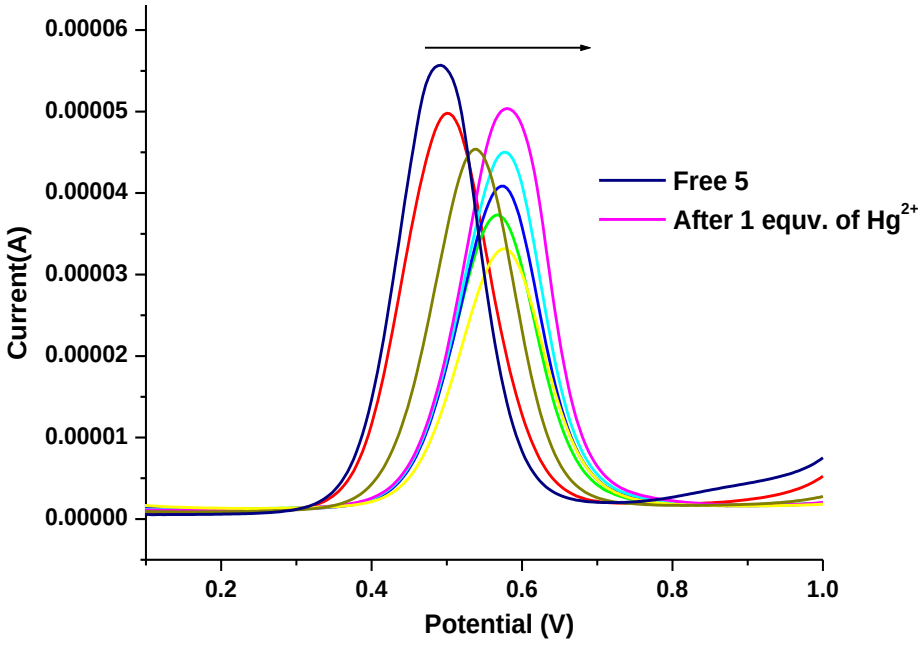



**Figure S10**. Evolution of DPV of **5** ($1x10^{-4}$ M) upon addition of $Hg^{2+}$ up to 1 equiv with $[(n\text{-}Bu)_4N]ClO_4$ as supporting electrolyte. Scan rate employed 0.1 $Vs^{-1}$.

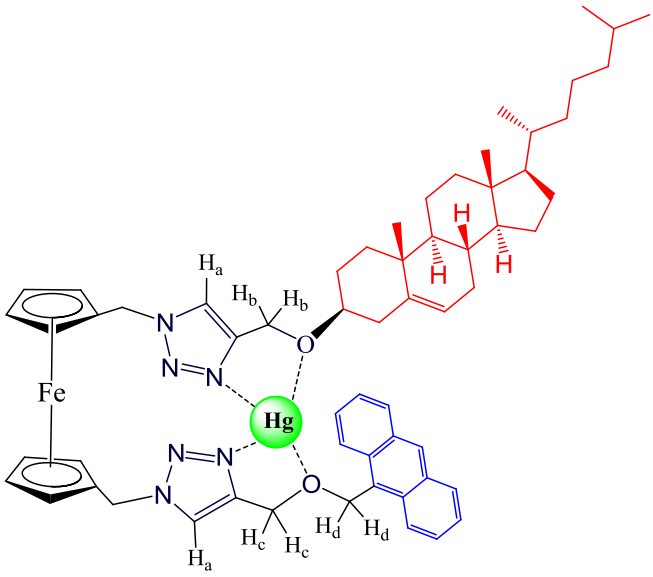



**Figure S11.** A plausible binding mode for **4** with $Hg^{2+}$ ion.

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

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | 4.82936200 | -0.95023500 | -1.67721600 | H | 5.68991100 | -1.94344500 | 1.49366100 |
| C | 3.23574900 | -0.39025600 | -2.85945900 | C | 11.84588400 | 0.22226700 | 1.44606900 |
| H | 3.28312300 | 0.39212700 | -3.60393900 | H | 11.15376200 | -0.47697100 | 0.97020800 |
| C | 6.27790800 | -0.78778400 | -0.22234600 | H | 12.62484900 | -0.39078400 | 1.92237200 |
| C | 6.16046400 | 0.43906200 | -0.94027300 | C | 15.32029600 | 2.48026400 | 2.44991600 |
| H | 5.87660900 | 1.39412800 | -0.51830100 | H | 15.71838200 | 2.41823200 | 3.45804500 |
| C | 6.43423400 | 0.17920500 | -2.30847500 | C | 10.71401000 | 0.67407400 | -1.28002500 |
| H | 6.38524300 | 0.89952200 | -3.11306900 | H | 10.15075500 | 0.06288500 | -0.58544700 |
| C | 6.63578100 | -1.80262500 | -1.15699400 | C | 15.48411100 | 3.39134000 | 0.22579900 |
| H | 6.78228400 | -2.84865100 | -0.92407000 | H | 15.97561900 | 4.00967800 | -0.52017300 |
| O | 11.17275600 | 0.98072200 | 2.44087300 | C | 15.98794600 | 3.28532000 | 1.48464900 |
| C | 14.29373500 | 2.69645900 | -0.15110400 | H | 16.89236600 | 3.81757600 | 1.76213800 |
| N | 7.38767800 | -0.93773200 | 1.97103300 | C | 12.06432600 | 2.28754300 | -3.12185100 |
| C | 13.62859600 | 1.86604200 | 0.80889800 | H | 12.59878500 | 2.91969700 | -3.82555800 |
| C | 6.72908400 | -1.20619700 | -2.44151600 | C | 10.91802000 | 1.65478900 | -3.48613900 |
| H | 6.94155600 | -1.72419300 | -3.36641100 | H | 10.52008400 | 1.76952500 | -4.48963200 |
| C | 11.92642700 | 1.30843700 | -0.84968500 | C | 10.23066600 | 0.84100700 | -2.54210000 |
| C | 14.18554200 | 1.79965400 | 2.12673600 | H | 9.30607500 | 0.35023900 | -2.82884100 |
| H | 13.66947500 | 1.22744300 | 2.88714600 | C | 10.52722100 | 0.17567400 | 3.40516100 |
| C | 12.47082500 | 1.15344600 | 0.43947900 | H | 10.29758800 | 0.84764700 | 4.23762400 |
| N | 8.94595100 | -1.75476600 | 3.16998400 | H | 11.19091300 | -0.61409700 | 3.78459500 |
| C | 3.40684600 | -2.43905600 | -1.82889500 | C | 2.70783000 | -1.79245900 | 0.58864400 |
| H | 3.58179000 | -3.49077300 | -1.64755500 | N | 1.40159100 | -2.41566700 | 0.74764300 |
| C | 12.60071300 | 2.14599400 | -1.80402600 | H | 3.41692400 | -2.50940300 | 1.00518100 |
| C | 9.27649300 | -0.46730100 | 2.88690900 | N | 1.32367400 | -3.74524800 | 0.89136700 |
| N | 7.80455500 | -2.03397100 | 2.62073500 | C | 0.16648100 | -1.86488200 | 0.69293400 |
| C | 13.76757400 | 2.80741500 | -1.43524700 | N | 0.06648900 | -4.06292300 | 0.93966200 |
| H | 14.27711200 | 3.43066700 | -2.16608100 | C | -0.68007000 | -2.93481200 | 0.82209000 |
| C | 2.91119300 | -0.21816900 | -1.48819200 | H | -0.01376600 | -0.80982000 | 0.57123900 |
| H | 2.65769000 | 0.71669900 | -1.00582700 | C | -2.17215700 | -2.95778600 | 0.84785400 |
| C | 3.02191200 | -1.48482200 | -0.84370900 | H | -2.54140900 | -3.64942300 | 0.07788500 |
| C | 8.27910300 | 0.06860600 | 2.10786300 | H | -2.52863300 | -3.33790100 | 1.81812700 |
| H | 8.15036400 | 1.03879800 | 1.65478400 | H | 2.73550400 | -0.88531900 | 1.19864300 |
| C | 3.53907600 | -1.76333100 | -3.06924100 | O | -2.62831800 | -1.64270800 | 0.63505200 |
| H | 3.85763600 | -2.20689300 | -4.00220300 | C | -4.02631400 | -1.46364400 | 0.78367900 |
| C | 6.11757200 | -0.96877400 | 1.25478600 | C | -4.28114200 | 0.02682800 | 0.92758000 |
| H | 5.46385100 | -0.19602600 | 1.67049900 | C | -4.81040800 | -2.01377500 | -0.41040500 |

| | | | |
|---|---|---|---|
| H | -4.35984400 | -1.97790900 | 1.70053300 |
| C | -5.77542100 | 0.31700500 | 1.06929100 |
| H | -3.86117500 | 0.53525500 | 0.05164900 |
| H | -3.73842200 | 0.40416900 | 1.80056800 |
| C | -6.28466200 | -1.68545600 | -0.32545300 |
| H | -4.68620800 | -3.09786900 | -0.49232400 |
| H | -4.36237600 | -1.57653100 | -1.31286100 |
| C | -6.65159500 | -0.21987800 | -0.09226500 |
| H | -5.92360700 | 1.39689400 | 1.17077500 |
| H | -6.12957500 | -0.13516500 | 2.00516200 |
| C | -7.19533000 | -2.65060700 | -0.44996000 |
| C | -8.14993600 | -0.09957500 | 0.31937200 |
| C | -6.34839000 | 0.57817700 | -1.37746000 |
| C | -8.67907700 | -2.44336000 | -0.42220500 |
| H | -6.85272000 | -3.67555200 | -0.58785800 |
| C | -9.07737700 | -0.97185900 | -0.55220000 |
| C | -8.64576200 | 1.35544500 | 0.40705800 |
| H | -8.21889500 | -0.52183300 | 1.33463600 |
| H | -6.40872700 | 1.65646600 | -1.20348800 |
| H | -5.34351300 | 0.36859100 | -1.75149700 |
| H | -7.04871300 | 0.32090900 | -2.17744000 |
| H | -9.08480800 | -2.85207700 | 0.51658900 |
| H | -9.14637100 | -3.03236100 | -1.22116300 |
| C | -10.52911300 | -0.76574800 | -0.12698600 |
| H | -8.96215300 | -0.68261400 | -1.60524400 |
| C | -10.12884700 | 1.49045100 | 0.78321500 |
| H | -8.48273500 | 1.86252100 | -0.54911500 |
| H | -8.04876600 | 1.90466300 | 1.14283100 |
| C | -11.03152400 | 0.69500100 | -0.17090800 |
| C | -11.62150300 | -1.56359000 | -0.83875500 |
| H | -10.57454600 | -1.05375500 | 0.93647700 |
| H | -10.28302600 | 1.11654400 | 1.80487800 |
| H | -10.38778400 | 2.55280300 | 0.79950800 |
| C | -12.51004800 | 0.48855000 | 0.27944100 |
| C | -10.98864200 | 1.28796900 | -1.58933500 |
| C | -12.92421100 | -0.83520400 | -0.43385400 |
| H | -11.62658100 | -2.61797500 | -0.54830000 |
| H | -11.47359100 | -1.53677700 | -1.92444600 |
| H | -12.47748600 | 0.29615200 | 1.36259600 |
| C | -13.53506200 | 1.62006700 | 0.05764200 |
| H | -9.98733000 | 1.25799900 | -2.02477200 |
| H | -11.30476900 | 2.33568800 | -1.57962300 |
| H | -11.65450000 | 0.75522500 | -2.27453500 |
| H | -13.53750600 | -1.45756900 | 0.22304200 |
| H | -13.54006300 | -0.61780900 | -1.31360100 |
| C | -14.91969700 | 1.18834900 | 0.57871000 |
| H | -13.63001500 | 1.77978000 | -1.02624800 |
| C | -13.11353300 | 2.94554800 | 0.69942300 |
| H | -15.14725700 | 0.18136100 | 0.21277000 |
| H | -14.87642000 | 1.10925300 | 1.67490700 |
| C | -16.08145800 | 2.10233100 | 0.18231400 |
| H | -12.90603100 | 2.81333300 | 1.76798600 |
| H | -12.21714200 | 3.36173600 | 0.23572100 |
| H | -13.89929200 | 3.69999900 | 0.60630400 |
| C | -17.43312000 | 1.56143300 | 0.65080700 |
| H | -16.09604300 | 2.21291500 | -0.91136900 |
| H | -15.92872700 | 3.10655800 | 0.59028900 |
| H | -17.54345800 | 0.52976200 | 0.28983800 |
| H | -17.43926000 | 1.49925500 | 1.74884800 |
| C | -18.65489400 | 2.36939100 | 0.19303400 |
| C | -19.94642400 | 1.64652900 | 0.57965100 |
| H | -18.61949100 | 2.43460300 | -0.90413200 |
| C | -18.65520600 | 3.79433700 | 0.75074600 |
| H | -20.82855400 | 2.18964100 | 0.22457600 |
| H | -19.98049800 | 0.63635000 | 0.15799100 |
| H | -20.02941300 | 1.55516600 | 1.66934200 |
| H | -18.65133500 | 3.78019600 | 1.84759400 |
| H | -17.78350300 | 4.36671700 | 0.42086800 |
| H | -19.54885600 | 4.33990400 | 0.42981100 |

Cartesian coordinates for the calculated structure of ligand **5** (in Å).

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | 4.29622400 | 1.40018200 | 1.73142700 | C | -0.45803300 | 2.24419900 | -0.48436700 |
| C | 2.75714100 | 0.70099100 | 2.91257200 | N | -0.67981000 | 4.44614400 | -0.54867300 |
| H | 2.85282200 | -0.12548500 | 3.60288300 | C | -1.36280100 | 3.27308900 | -0.51345800 |
| C | 5.71065300 | 1.40934800 | 0.23766500 | H | -0.57941200 | 1.17447000 | -0.44662100 |
| C | 5.65982100 | 0.12620700 | 0.85858000 | C | -2.85421900 | 3.21659300 | -0.51875300 |
| H | 5.40147100 | -0.80348500 | 0.36865600 | H | -3.24745600 | 3.83741500 | 0.29808800 |
| C | 5.96033700 | 0.28935100 | 2.23609300 | H | -3.24602200 | 3.63691900 | -1.45839600 |
| H | 5.96217300 | -0.49278400 | 2.98230900 | H | 2.14401400 | 1.44147300 | -1.09386200 |
| C | 6.05437000 | 2.36119200 | 1.24133900 | O | -3.23688500 | 1.86802000 | -0.38469300 |
| H | 6.15528600 | 3.42720000 | 1.08830800 | C | -4.62049500 | 1.61965000 | -0.56380500 |
| O | 10.63654500 | 0.07000100 | -2.40203600 | C | -4.79254300 | 0.12395100 | -0.76375500 |
| N | 6.79234800 | 1.78917100 | -1.93276000 | C | -5.45336800 | 2.08418000 | 0.63351400 |
| C | 6.20512400 | 1.66993000 | 2.47138900 | H | -4.96633200 | 2.14776900 | -1.46836600 |
| H | 6.42306100 | 2.12123100 | 3.42925600 | C | -6.26652600 | -0.23843500 | -0.94610700 |
| N | 8.32599500 | 2.78247700 | -3.02574400 | H | -4.36267100 | -0.39254000 | 0.10258900 |
| C | 2.82233000 | 2.81750200 | 2.01571800 | H | -4.21462100 | -0.19337600 | -1.63807100 |
| H | 2.95153400 | 3.88498100 | 1.90006800 | C | -6.90652400 | 1.68359400 | 0.50675000 |
| C | 8.73164900 | 1.50299700 | -2.81528300 | H | -5.38706000 | 3.16955800 | 0.75677600 |
| N | 7.15405400 | 2.95121500 | -2.49499700 | H | -4.99981300 | 1.63719600 | 1.52848000 |
| C | 2.40325900 | 0.60560400 | 1.54110300 | C | -7.19209100 | 0.21023200 | 0.21463300 |
| H | 2.17171300 | -0.30521500 | 1.00460400 | H | -6.35535600 | -1.32029900 | -1.08783500 |
| C | 2.44853700 | 1.91486800 | 0.97911600 | H | -6.62642100 | 0.22751100 | -1.87299500 |
| C | 7.75100000 | 0.85331600 | -2.10633700 | C | -7.86870300 | 2.59518700 | 0.64660600 |
| H | 7.67716500 | -0.14959100 | -1.71726100 | C | -8.67394200 | 0.02806500 | -0.23236500 |
| C | 3.01361700 | 2.06835900 | 3.20512300 | C | -6.87299700 | -0.61719900 | 1.47728500 |
| H | 3.33997900 | 2.46276900 | 4.15727600 | C | -9.33872100 | 2.31270900 | 0.58114200 |
| C | 5.52378000 | 1.69755400 | -1.21932700 | H | -7.58299000 | 3.63075300 | 0.82780000 |
| H | 4.90974100 | 0.92518800 | -1.69229400 | C | -9.66107000 | 0.81866900 | 0.65148500 |
| H | 5.04369700 | 2.66378000 | -1.38011500 | C | -9.09075100 | -1.44635900 | -0.38187900 |
| C | 11.19740700 | 0.70988000 | -1.26567300 | H | -8.74611100 | 0.48346700 | -1.23296000 |
| H | 10.44402800 | 1.33728800 | -0.77280900 | H | -6.87077000 | -1.68995300 | 1.26324100 |
| H | 12.01220400 | 1.37545200 | -1.59155200 | H | -5.88928500 | -0.36784100 | 1.88189300 |
| C | 10.04300000 | 0.97442800 | -3.31118100 | H | -7.60326100 | -0.42787500 | 2.26944100 |
| H | 9.90798400 | 0.40910700 | -4.23824000 | H | -9.74804900 | 2.73344700 | -0.35074000 |
| H | 10.70495100 | 1.82391900 | -3.53072400 | H | -9.85124600 | 2.84717500 | 1.39064300 |
| C | 2.08486300 | 2.30207500 | -0.42186700 | C | -11.09263800 | 0.55215500 | 0.19265600 |
| N | 0.74466500 | 2.86435100 | -0.51119000 | H | -9.54799800 | 0.49837500 | 1.69570500 |
| H | 2.74667000 | 3.08183800 | -0.80163800 | C | -10.55742000 | -1.64418700 | -0.79283000 |
| N | 0.59326200 | 4.19487400 | -0.54449400 | H | -8.91893600 | -1.97850000 | 0.55898400 |

| | | | |
|---|---|---|---|
| H | -8.45206200 | -1.93641500 | -1.12442600 |
| C | -11.51761200 | -0.93356000 | 0.17227700 |
| C | -12.23711000 | 1.26405300 | 0.91377500 |
| H | -11.13602700 | 0.87774900 | -0.85997500 |
| H | -10.71254800 | -1.24038500 | -1.80290700 |
| H | -10.75906100 | -2.71735600 | -0.85373200 |
| C | -12.99724700 | -0.78608200 | -0.29767300 |
| C | -11.46816400 | -1.57845800 | 1.56776200 |
| C | -13.49272400 | 0.48269100 | 0.46170300 |
| H | -12.29421000 | 2.32652100 | 0.66073200 |
| H | -12.10416100 | 1.20607100 | 2.00014300 |
| H | -12.95605600 | -0.54622000 | -1.37103100 |
| C | -13.96537900 | -1.97734500 | -0.14270300 |
| H | -10.47912400 | -1.50801200 | 2.02611500 |
| H | -11.72215300 | -2.64152400 | 1.51034200 |
| H | -12.17749600 | -1.11307100 | 2.25840400 |
| H | -14.13214900 | 1.09639300 | -0.17821800 |
| H | -14.10578900 | 0.19547200 | 1.32320400 |
| C | -15.36246100 | -1.59146500 | -0.66590900 |
| H | -14.06713200 | -2.19036300 | 0.93138300 |
| C | -13.46619700 | -3.24941700 | -0.83424100 |
| H | -15.65541500 | -0.62764200 | -0.23569300 |
| H | -15.30209600 | -1.43196700 | -1.75253400 |
| C | -16.47707300 | -2.59555000 | -0.36338200 |
| H | -13.26069600 | -3.06277400 | -1.89510300 |
| H | -12.54980500 | -3.63090600 | -0.38017200 |
| H | -14.20734600 | -4.05104300 | -0.77670500 |
| C | -17.85144800 | -2.08769700 | -0.80204300 |
| H | -16.49568100 | -2.80049300 | 0.71656200 |
| H | -16.26800300 | -3.55136500 | -0.85389300 |
| H | -18.02280800 | -1.10132800 | -0.34978400 |
| H | -17.84903700 | -1.92490900 | -1.88978100 |
| C | -19.03090200 | -3.00052400 | -0.44049700 |
| C | -20.35712600 | -2.31464400 | -0.77332400 |
| H | -19.00105600 | -3.16970600 | 0.64567600 |
| C | -18.94926100 | -4.36266600 | -1.13295200 |
| H | -21.21060700 | -2.93754100 | -0.48560700 |
| H | -20.45146200 | -1.35412500 | -0.25581300 |
| H | -20.43529600 | -2.12173400 | -1.85004100 |
| H | -18.93720700 | -4.24213600 | -2.22320300 |
| H | -18.05105800 | -4.91824300 | -0.84835700 |
| H | -19.81512600 | -4.98286200 | -0.87825000 |
| C | 11.70420800 | -0.32161700 | -0.29383800 |
| C | 12.76579200 | -1.18440900 | -0.62647800 |
| C | 11.12752900 | -0.40472500 | 0.96978300 |
| C | 13.23967700 | -2.11017200 | 0.34152600 |
| C | 13.40368300 | -1.16231900 | -1.91775300 |
| C | 11.57977400 | -1.31131100 | 1.91777100 |
| H | 10.30574400 | 0.26160100 | 1.21768600 |
| C | 14.32876100 | -2.98084100 | 0.03143200 |
| C | 12.63717300 | -2.17229900 | 1.62645600 |
| C | 14.43709000 | -1.98522100 | -2.20748000 |
| H | 13.01632100 | -0.48971800 | -2.67274800 |
| H | 11.11279600 | -1.35352200 | 2.89763800 |
| C | 14.94252800 | -2.92505900 | -1.24601700 |
| C | 14.80430200 | -3.90411400 | 1.00009700 |
| C | 13.13823800 | -3.11939000 | 2.58678900 |
| H | 14.90286500 | -1.95425800 | -3.18854200 |
| C | 16.00890300 | -3.78312400 | -1.53037100 |
| C | 15.87234600 | -4.74356400 | 0.67539400 |
| C | 14.16771900 | -3.94255100 | 2.28979800 |
| H | 12.66596500 | -3.15568500 | 3.56447700 |
| C | 16.46813200 | -4.68246100 | -0.57818500 |
| H | 16.47641300 | -3.73833900 | -2.50991800 |
| H | 16.23509600 | -5.44873700 | 1.41790800 |
| H | 14.53745100 | -4.65240100 | 3.02436000 |
| H | 17.29747800 | -5.34201600 | -0.81395200 |

Cartesian coordinates for the calculated structure of ligand **4.Hg**$^{2+}$ (in Å).

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | -7.92672200 | -3.00602200 | -1.08714900 | H | -0.68231700 | 3.11214900 | -1.14777700 |
| C | -7.80682000 | -5.08255900 | -0.96905600 | H | -0.62596400 | 2.94711300 | 0.61275800 |
| H | -8.52269500 | -5.75467100 | -1.42345100 | C | -2.32611800 | 4.96888600 | 3.61383200 |
| C | -8.29259400 | -0.94358000 | -1.23306500 | H | -2.42789300 | 4.30376400 | 4.46650400 |
| C | -9.45941900 | -1.63565000 | -0.76394700 | C | -1.07021000 | 5.28397500 | -2.49871800 |
| H | -9.96695400 | -1.46029900 | 0.17670600 | H | -0.88513300 | 4.24082800 | -2.72903000 |
| C | -9.84768400 | -2.57179800 | -1.76384000 | C | -2.39242600 | 7.20488700 | 2.71629700 |
| H | -10.67811500 | -3.26205200 | -1.69716600 | H | -2.53470300 | 8.27569200 | 2.83232600 |
| C | -7.96063800 | -1.47350100 | -2.51834900 | C | -2.51700500 | 6.36147500 | 3.79310200 |
| H | -7.11792100 | -1.18260600 | -3.13203000 | H | -2.76094100 | 6.75284300 | 4.77543500 |
| O | -2.43686000 | 2.49996400 | -0.18249300 | C | -1.50839600 | 8.01600400 | -2.04171100 |
| C | -2.06812700 | 6.69776700 | 1.42345000 | H | -1.67601500 | 9.07169500 | -1.84743000 |
| N | -6.36924200 | 0.66715400 | -0.85400400 | C | -1.19014900 | 7.57903100 | -3.30412100 |
| C | -1.86312300 | 5.28251400 | 1.23331200 | H | -1.10214100 | 8.28147100 | -4.12652900 |
| C | -8.91861500 | -2.47843800 | -2.84017500 | C | -0.97017200 | 6.19743100 | -3.52648800 |
| H | -8.91559100 | -3.09079600 | -3.73225800 | H | -0.71374400 | 5.85206400 | -4.52370400 |
| C | -1.39881300 | 5.68735600 | -1.16938100 | C | -3.39982100 | 2.76550000 | -1.24268100 |
| C | -2.02100900 | 4.44489200 | 2.37552500 | H | -2.89966300 | 2.64796800 | -2.21236700 |
| H | -1.91340100 | 3.36998900 | 2.27956900 | H | -3.75885700 | 3.79293600 | -1.15567800 |
| C | -1.50862500 | 4.79376500 | -0.06086400 | C | -6.43262100 | -3.01609500 | 1.86610700 |
| N | -4.26357300 | 0.47837100 | -0.85060300 | N | -5.00538800 | -2.64870800 | 1.94113400 |
| C | -6.00360900 | -3.67513400 | -0.66544100 | H | -6.96949200 | -2.08433000 | 2.05301200 |
| H | -5.11004400 | -3.09666600 | -0.85480000 | N | -4.66875800 | -1.36459600 | 1.99597900 |
| C | -1.62232400 | 7.09991000 | -0.95471000 | C | -3.90980300 | -3.44920700 | 1.81982800 |
| C | -4.52597600 | 1.79286600 | -1.09252200 | N | -3.35817200 | -1.32471700 | 1.92803300 |
| N | -5.37386800 | -0.19881200 | -0.68495000 | C | -2.84104900 | -2.58081800 | 1.79863400 |
| C | -1.94350000 | 7.56032100 | 0.32775200 | H | -3.98072100 | -4.52323000 | 1.73951200 |
| H | -2.10338900 | 8.62563800 | 0.47727000 | C | -1.36728900 | -2.76461400 | 1.61786100 |
| C | -7.89503600 | -4.53874200 | 0.34429800 | H | -0.83430600 | -2.55356900 | 2.55188700 |
| H | -8.67715600 | -4.74326200 | 1.06503700 | H | -1.14773200 | -3.78926600 | 1.30814700 |
| C | -6.77519500 | -3.67189500 | 0.54488700 | H | -6.64417400 | -3.69672500 | 2.69712100 |
| C | -5.89776000 | 1.92096000 | -1.10640700 | O | -0.93541100 | -1.84309100 | 0.58635200 |
| H | -6.54967800 | 2.76757400 | -1.25989000 | C | 0.52358100 | -1.66046100 | 0.41476800 |
| C | -6.63762900 | -4.55542000 | -1.59020700 | C | 1.11638900 | -0.75747900 | 1.48741200 |
| H | -6.30839500 | -4.75630200 | -2.60117600 | C | 1.28064000 | -2.98855800 | 0.32127800 |
| C | -7.77120900 | 0.29132900 | -0.55747300 | H | 0.57174500 | -1.16099200 | -0.55874500 |
| H | -8.36190400 | 1.16289800 | -0.86076700 | C | 2.60251400 | -0.49011400 | 1.18578600 |
| H | -7.85175900 | 0.20656800 | 0.53133500 | H | 1.00441400 | -1.21195700 | 2.47971200 |
| C | -1.20990500 | 3.34391600 | -0.22174500 | H | 0.56563600 | 0.19946500 | 1.51027400 |

| | | | |
|---|---|---|---|
| C | 2.75321100 | -2.71574500 | 0.05394400 |
| H | 0.85850600 | -3.60930700 | -0.47631400 |
| H | 1.16689600 | -3.53913400 | 1.26524500 |
| C | 3.47194600 | -1.77898900 | 1.03065000 |
| H | 3.01450500 | 0.14333700 | 1.97734500 |
| H | 2.66766900 | 0.08660700 | 0.25292100 |
| C | 3.35574200 | -3.29490100 | -0.99444700 |
| C | 4.86732000 | -1.35377000 | 0.44633400 |
| C | 3.61462500 | -2.48135300 | 2.40576900 |
| C | 4.81366200 | -3.16446400 | -1.32006000 |
| H | 2.76304100 | -3.92396900 | -1.65990500 |
| C | 5.63819600 | -2.54573500 | -0.17974300 |
| C | 5.73831700 | -0.56187000 | 1.44924300 |
| H | 4.64747900 | -0.67326600 | -0.39328500 |
| H | 3.95968700 | -1.78632000 | 3.17727800 |
| H | 2.66671800 | -2.90465200 | 2.75502600 |
| H | 4.32957500 | -3.30762200 | 2.34963500 |
| H | 4.91932200 | -2.55341100 | -2.23210600 |
| H | 5.21302900 | -4.15098400 | -1.58871000 |
| C | 7.00480200 | -2.06526800 | -0.68922000 |
| H | 5.78909700 | -3.32057400 | 0.58469500 |
| C | 7.12221800 | -0.16296800 | 0.89581100 |
| H | 5.88538100 | -1.15156300 | 2.36012300 |
| H | 5.21200700 | 0.34956400 | 1.76118400 |
| C | 7.90720400 | -1.38585200 | 0.37932000 |
| C | 7.92981000 | -3.07366000 | -1.38580600 |
| H | 6.78846000 | -1.27620500 | -1.43070900 |
| H | 6.99378100 | 0.55052100 | 0.06864200 |
| H | 7.66541900 | 0.36972400 | 1.68234700 |
| C | 9.17592700 | -1.08117400 | -0.49142800 |
| C | 8.26992200 | -2.34121300 | 1.53841600 |
| C | 9.30678400 | -2.35427800 | -1.39628500 |
| H | 7.58894100 | -3.33037500 | -2.39437300 |
| H | 7.97784800 | -4.01273600 | -0.82046100 |
| H | 8.90486500 | -0.23253900 | -1.13997900 |
| C | 10.51105400 | -0.70540400 | 0.20303900 |
| H | 7.38862900 | -2.76442400 | 2.03065900 |
| H | 8.84669500 | -1.81649800 | 2.30712100 |
| H | 8.87982700 | -3.18308600 | 1.19686100 |
| H | 9.60081500 | -2.08088500 | -2.41366200 |
| H | 10.09322100 | -3.01621600 | -1.01601600 |
| C | 11.60769300 | -0.44222200 | -0.85984700 |
| H | 10.83591300 | -1.57247600 | 0.79838600 |
| C | 10.38308700 | 0.50075500 | 1.14984000 |
| H | 11.59114900 | -1.24515400 | -1.60665700 |
| H | 11.35762200 | 0.48190900 | -1.40429100 |
| C | 13.04187000 | -0.34054400 | -0.31577800 |
| H | 9.96867900 | 1.37154400 | 0.62487300 |
| H | 9.74059900 | 0.28989300 | 2.00954400 |
| H | 11.35827100 | 0.79306300 | 1.55045900 |
| C | 14.08020900 | -0.14796400 | -1.43152800 |
| H | 13.27959500 | -1.25653700 | 0.24617400 |
| H | 13.11761600 | 0.48651300 | 0.39929300 |
| H | 13.95371800 | -0.95112900 | -2.17257500 |
| H | 13.86959900 | 0.79186900 | -1.96543600 |
| C | 15.55137000 | -0.13922500 | -0.96848100 |
| C | 16.49340700 | -0.11429500 | -2.18203000 |
| H | 15.73323100 | -1.07702500 | -0.42055800 |
| C | 15.86550300 | 1.02952200 | -0.02114800 |
| H | 17.54366700 | -0.15101600 | -1.87040500 |
| H | 16.31090500 | -0.96566200 | -2.84865400 |
| H | 16.35316200 | 0.80388400 | -2.76744000 |
| H | 15.66653500 | 1.99254700 | -0.51041700 |
| H | 15.26966000 | 0.99136100 | 0.89739100 |
| H | 16.92156700 | 1.02059500 | 0.27264900 |
| Hg | -2.33517500 | 0.17872500 | 0.48871800 |

Cartesian coordinates for the calculated structure of ligand **5.Hg**$^{2+}$ (in Å).

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | 7.79436400 | -3.48219700 | 1.15468600 | C | 3.65273100 | -4.21794700 | -1.57873100 |
| C | 7.50158400 | -5.52397200 | 1.45203000 | N | 3.20477100 | -2.08941200 | -1.88923100 |
| H | 8.17738900 | -6.15447000 | 2.01462100 | C | 2.62943400 | -3.29746800 | -1.62412200 |
| C | 8.26082600 | -1.44352200 | 0.96388300 | H | 3.67212900 | -5.28068900 | -1.39074200 |
| C | 9.34232200 | -2.25953100 | 0.48815100 | C | 1.15271000 | -3.38866300 | -1.40400400 |
| H | 9.75568500 | -2.24527300 | -0.51302300 | H | 0.61251100 | -3.25072800 | -2.34774600 |
| C | 9.79372900 | -3.06841100 | 1.56898600 | H | 0.89174100 | -4.36444400 | -0.98702000 |
| H | 10.58216600 | -3.80774200 | 1.52112200 | H | 6.33840700 | -4.74948400 | -2.39934200 |
| C | 8.04525300 | -1.76947600 | 2.33879700 | O | 0.78489300 | -2.34621700 | -0.46823200 |
| H | 7.28537200 | -1.34798000 | 2.98432300 | C | -0.65962500 | -2.07997200 | -0.29328400 |
| O | 2.44277700 | 2.01817600 | -0.27933500 | C | -1.21756800 | -1.22035500 | -1.41886700 |
| N | 6.36056500 | 0.17703000 | 0.48277200 | C | -1.48050400 | -3.35957500 | -0.10650900 |
| C | 8.98863400 | -2.77241500 | 2.70682700 | H | -0.67158100 | -1.51524500 | 0.64506300 |
| H | 9.05344900 | -3.25323800 | 3.67406800 | C | -2.68793900 | -0.86494800 | -1.13405100 |
| N | 4.25231200 | 0.05774800 | 0.59114700 | H | -1.12882800 | -1.74062200 | -2.38063300 |
| C | 5.80918100 | -4.05064700 | 0.91571000 | H | -0.62082100 | -0.29401400 | -1.50165600 |
| H | 4.97871400 | -3.36454100 | 1.00485700 | C | -2.93936600 | -3.00480700 | 0.13668400 |
| C | 4.55913300 | 1.38438900 | 0.62584200 | H | -1.08663400 | -3.94164600 | 0.73365900 |
| N | 5.33652900 | -0.67119100 | 0.48287500 | H | -1.39587900 | -3.98173900 | -1.00809000 |
| C | 7.58417600 | -5.25583500 | 0.05543900 | C | -3.61499500 | -2.10087500 | -0.90017600 |
| H | 8.31960500 | -5.66325800 | -0.62728000 | H | -3.07299300 | -0.26288000 | -1.96294600 |
| C | 6.53282000 | -4.34896100 | -0.28727400 | H | -2.72334600 | -0.22961900 | -0.23838900 |
| C | 5.93294700 | 1.46899400 | 0.56596300 | C | -3.56963600 | -3.49488200 | 1.21354900 |
| H | 6.61269800 | 2.30756200 | 0.56627400 | C | -4.99147800 | -1.58102400 | -0.34714500 |
| C | 6.40360600 | -4.78577700 | 1.98193600 | C | -3.78706200 | -2.88033000 | -2.22964600 |
| H | 6.09852800 | -4.75623400 | 3.01965100 | C | -5.02287700 | -3.28842000 | 1.51900300 |
| C | 7.73547600 | -0.28131400 | 0.17218800 | H | -3.00592400 | -4.10580300 | 1.91980000 |
| H | 8.36515900 | 0.60000600 | 0.33771200 | C | -5.81425800 | -2.70520600 | 0.33729300 |
| H | 7.75714800 | -0.50088100 | -0.90024400 | C | -5.82417700 | -0.80508200 | -1.39409400 |
| C | 1.23848900 | 2.89666100 | -0.29112200 | H | -4.74330800 | -0.86730500 | 0.45627500 |
| H | 0.79217500 | 2.85856100 | 0.70520000 | H | -4.11336300 | -2.22240000 | -3.04087700 |
| H | 0.58087600 | 2.37587300 | -0.99307900 | H | -2.85519200 | -3.35443900 | -2.55651700 |
| C | 3.46664700 | 2.40458700 | 0.68023300 | H | -4.52766200 | -3.67819600 | -2.12164600 |
| H | 3.01539900 | 2.44614600 | 1.67998700 | H | -5.11034500 | -2.62179300 | 2.39324200 |
| H | 3.84569500 | 3.39657400 | 0.42549600 | H | -5.46238800 | -4.24147200 | 1.84090400 |
| C | 6.19109700 | -3.92111000 | -1.69931100 | C | -7.16520100 | -2.14757100 | 0.80606700 |
| N | 4.78308600 | -3.49195800 | -1.80406500 | H | -5.98883300 | -3.51603300 | -0.38379200 |
| H | 6.77210100 | -3.07062000 | -2.06058000 | C | -7.19645100 | -0.32729400 | -0.87411800 |
| N | 4.50932700 | -2.20356500 | -1.98002300 | H | -5.98645800 | -1.43110100 | -2.27790500 |

| | | | |
|---|---|---|---|
| H | -5.26070900 | 0.06989800 | -1.74345100 |
| C | -8.03210000 | -1.49154500 | -0.30495500 |
| C | -8.13231200 | -3.08481300 | 1.54337900 |
| H | -6.92550700 | -1.32978700 | 1.50834500 |
| H | -7.04706700 | 0.42135000 | -0.08222600 |
| H | -7.71222400 | 0.18599700 | -1.69146700 |
| C | -9.29678600 | -1.09709600 | 0.53621100 |
| C | -8.41962300 | -2.49038000 | -1.41832900 |
| C | -9.48204600 | -2.31720200 | 1.50219600 |
| H | -7.80984000 | -3.30173200 | 2.56717600 |
| H | -8.20945100 | -4.04918700 | 1.02567000 |
| H | -9.00023700 | -0.22722000 | 1.14424400 |
| C | -10.61085200 | -0.70847900 | -0.19082600 |
| H | -7.54923900 | -2.96705500 | -1.88010400 |
| H | -8.97204600 | -1.98537000 | -2.21762600 |
| H | -9.06099400 | -3.29251100 | -1.04064000 |
| H | -9.77501200 | -1.98203000 | 2.50128100 |
| H | -10.28871900 | -2.96938400 | 1.14825900 |
| C | -11.71089000 | -0.36873900 | 0.84636100 |
| H | -10.95645900 | -1.58900800 | -0.75398600 |
| C | -10.43318300 | 0.45251400 | -1.18444400 |
| H | -11.74271100 | -1.15423800 | 1.61100700 |
| H | -11.42701900 | 0.55534500 | 1.37407800 |
| C | -13.13092800 | -0.21379500 | 0.27810300 |
| H | -10.00396400 | 1.33328900 | -0.68878600 |
| H | -9.78192700 | 0.18797900 | -2.02236400 |
| H | -11.39262000 | 0.75378600 | -1.61527000 |
| C | -14.17912000 | 0.01456800 | 1.37790200 |
| H | -13.39371300 | -1.11941400 | -0.28954000 |
| H | -13.16497400 | 0.61692100 | -0.43568800 |
| H | -14.09636700 | -0.79688400 | 2.11595700 |
| H | -13.94026000 | 0.94244900 | 1.92077400 |
| C | -15.64110900 | 0.08381700 | 0.89155800 |
| C | -16.60115600 | 0.13245600 | 2.09024900 |
| H | -15.84937200 | -0.84093500 | 0.33098000 |
| C | -15.89609500 | 1.27310100 | -0.04781500 |
| H | -17.64686400 | 0.13886900 | 1.76163000 |
| H | -16.46213300 | -0.73172800 | 2.75086600 |
| H | -16.43579300 | 1.03888200 | 2.68733700 |
| H | -15.67071500 | 2.22299100 | 0.45541300 |
| H | -15.28672000 | 1.22309700 | -0.95692500 |
| H | -16.94663700 | 1.30592900 | -0.35926700 |
| Hg | 2.26954200 | -0.37511100 | -0.63137700 |
| C | 1.56472000 | 4.26934600 | -0.76557200 |
| C | 1.76176500 | 4.44470600 | -2.14961000 |
| C | 1.68780300 | 5.38902100 | 0.11198400 |
| C | 2.07466700 | 5.67717100 | -2.68967100 |
| H | 1.64874500 | 3.58729500 | -2.80876200 |
| C | 2.00978400 | 6.66875600 | -0.44963200 |
| C | 1.49965700 | 5.31207400 | 1.53154300 |
| C | 2.20616300 | 6.81249800 | -1.85908100 |
| H | 2.20733800 | 5.78670300 | -3.76208600 |
| C | 2.13415600 | 7.81347800 | 0.39134300 |
| C | 1.62019600 | 6.41459600 | 2.33520400 |
| H | 1.24010200 | 4.36596600 | 1.99421000 |
| C | 2.52036500 | 8.09800600 | -2.39629400 |
| C | 2.44927600 | 9.08793500 | -0.17019100 |
| C | 1.94117400 | 7.69739500 | 1.79901700 |
| H | 1.46233400 | 6.32246200 | 3.40651400 |
| C | 2.63731700 | 9.19354500 | -1.58384100 |
| H | 2.66298600 | 8.19296400 | -3.46887800 |
| C | 2.56364000 | 10.20393700 | 0.68128800 |
| C | 2.06519000 | 8.84204900 | 2.61347100 |
| H | 2.87445200 | 10.16546000 | -2.00765100 |
| H | 2.80271400 | 11.17291100 | 0.25176500 |
| C | 2.37316400 | 10.08065300 | 2.05788100 |
| H | 1.91418200 | 8.74824500 | 3.68544300 |
| H | 2.46374800 | 10.95370400 | 2.69619600 |

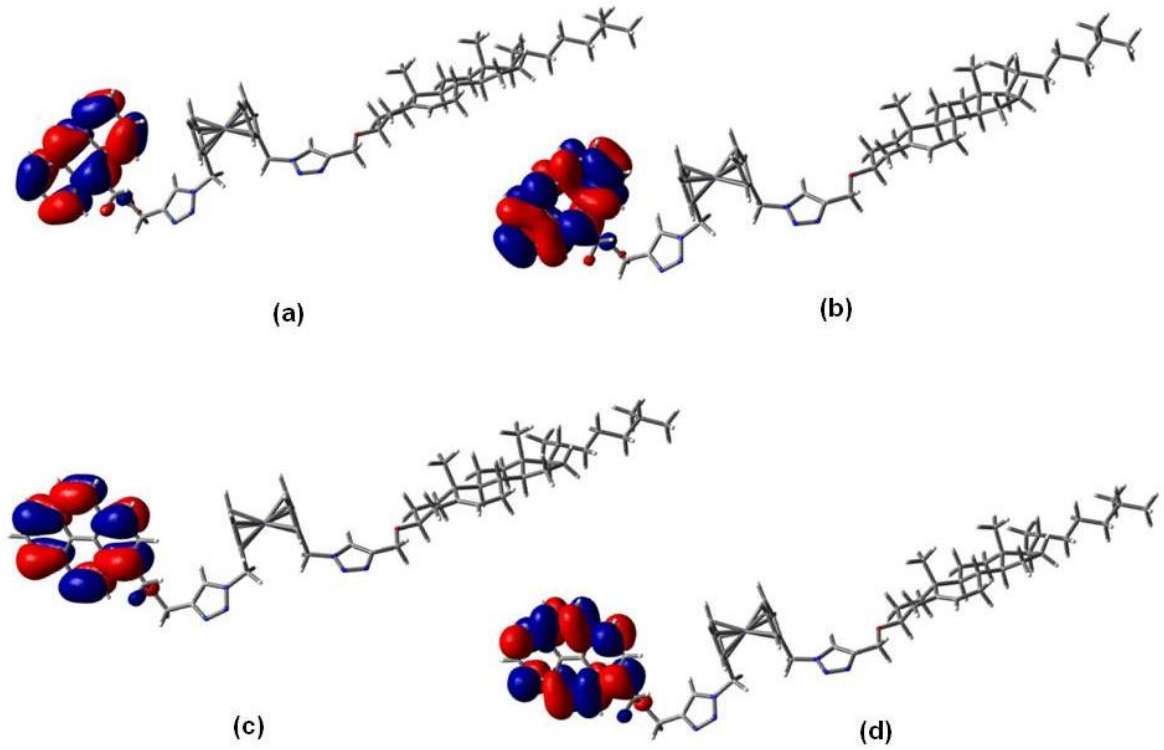



**Figure S12**. Pictorial representation of the molecular orbitals (MOs) present on different fragments of L: (a) HOMO of **4**; (b) LUMO of **4**; (c) HOMO of **5**; (d) LUMO of **5**.

**Table S1**. Distance of metal to donor center and Wiberg Bond Indices (WBI) of **4.Hg**$^{2+}$ and **5.Hg**$^{2+}$.

| **Compounds** | **Distances** (Å) | **WBI** |
|---|---|---|
| **4.Hg**$^{2+}$ | | |
| $d_{Hg-N}$ | 2.36924 | 0.2152 |
| $d_{Hg-N}$ | 2.32286 | 0.2454 |
| $d_{M-O\ (anthracene)}$ | 2.42524 | 0.2033 |
| $d_{M-O\ (cholesterol)}$ | 2.47307 | 0.1832 |
| **5.Hg**$^{2+}$ | | |
| $d_{Hg-N}$ | 2.36692 | 0.2188 |
| $d_{Hg-N}$ | 2.31916 | 0.2482 |
| $d_{M-O\ (pyrene)}$ | 2.41847 | 0.2039 |
| $d_{M-O\ (\ cholesterol\ )}$ | 2.46102 | 0.1834 |

**Table S2**. DFT calculated energies of HOMO and LUMO (eV), HOMO-LUMO gaps ($\Delta E = E_{LUMO} - E_{HOMO}$, eV) of **4**, **5**, **4.Hg$^{2+}$** and **5.Hg$^{2+}$**.

| Compound | **4** | **5** | **4.Hg$^{2+}$** | **5.Hg$^{2+}$** |
|---|---|---|---|---|
| HOMO | -5.23 | -5.34 | -9.65 | -9.59 |
| LUMO | -1.64 | -1.49 | -8.93 | -8.84 |
| ΔE | 3.59 | 3.85 | 0.72 | 0.75 |

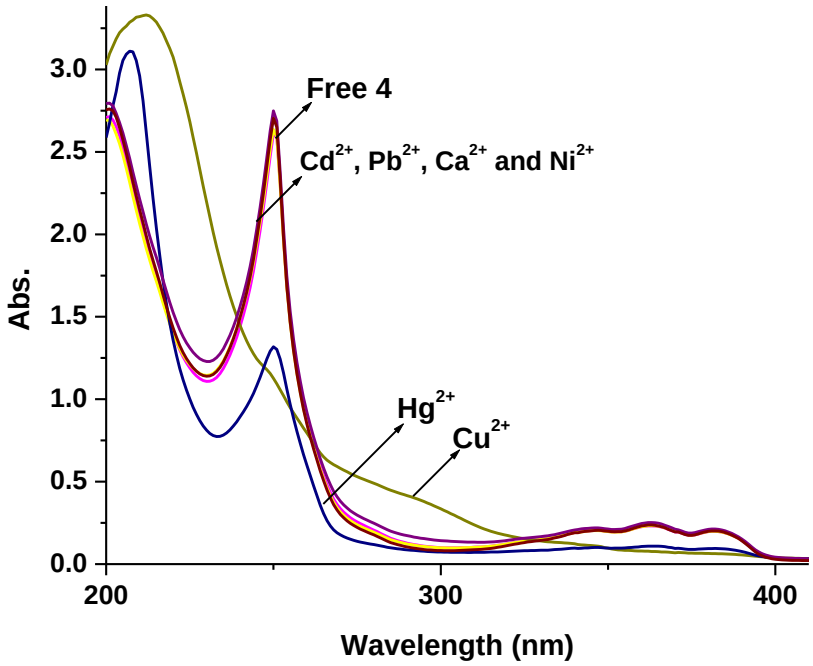



**Figure S13.** Changes in absorption spectra of **4** (1 x $10^{-5}$ M) in $CH_3CN/H_2O$ (5:5) upon addition of several metal cations.

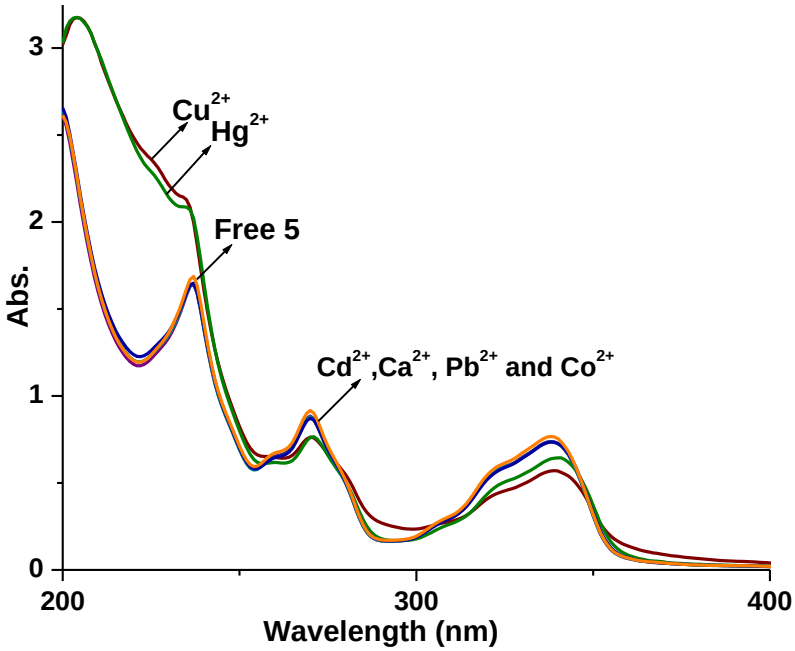



**Figure S14:** Changes in absorption spectra of **5** (1 x $10^{-5}$ M) in $CH_3CN/H_2O$ (5:5) upon addition of several metal cations.

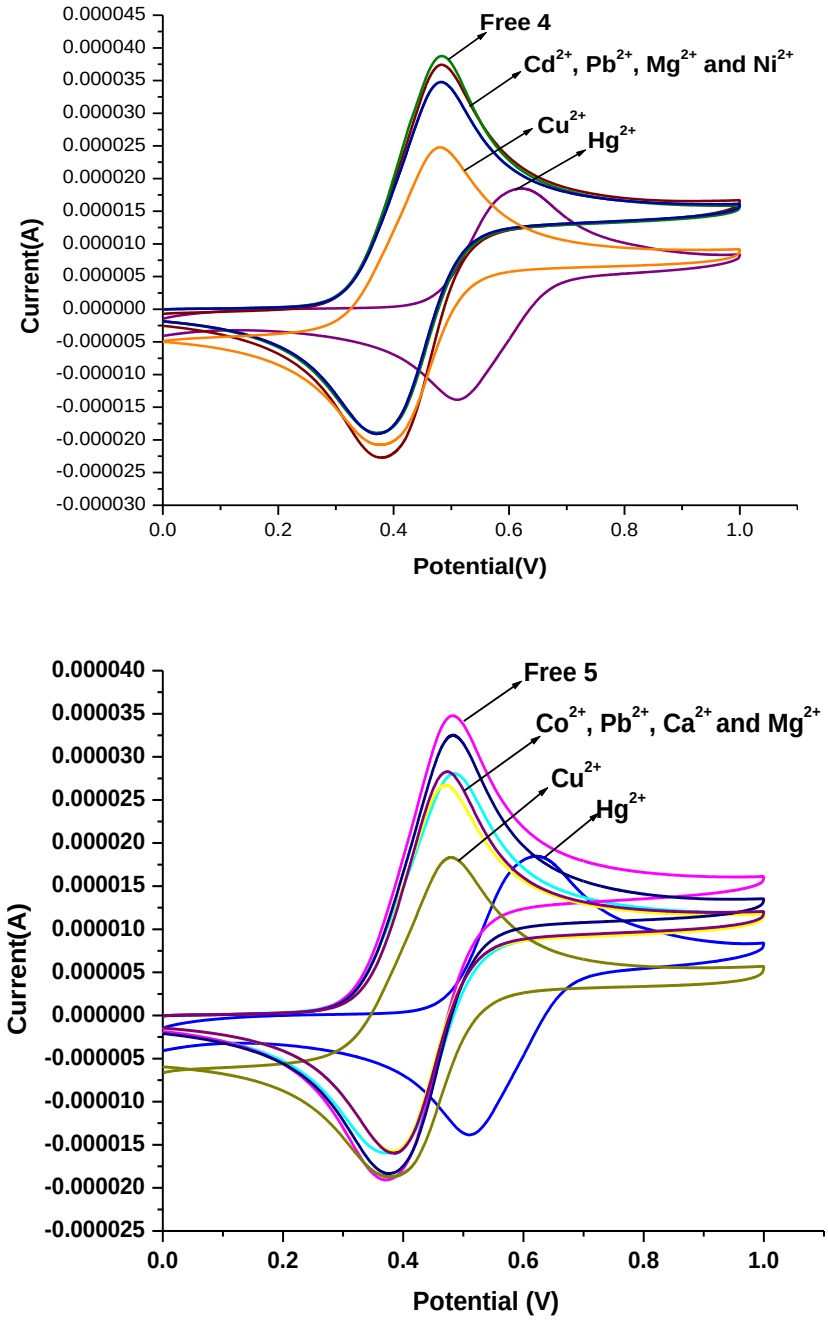



**Figure S15**. Evolution of CV of **4 (**top) and **5** (bottom) ($1x10^{-4}$ M) upon addition of several metal cations upto 1 equiv with $[(n\text{-}Bu)_4N]ClO_4$ as supporting electrolyte. Scan rate employed 0.1 $Vs^{-1}$.

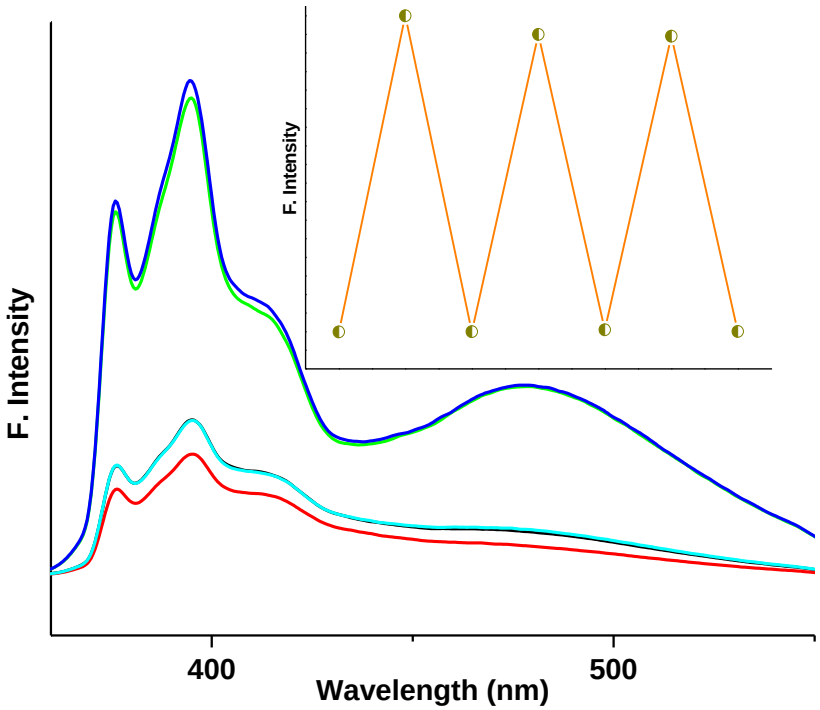



**Figure S16**. Reversibility of the interaction between **5** and $Hg^{2+}$ by the introduction of $I^-$ to the system. Inset: Stepwise complexation/decomplexation cycles carried out in ($1\times10^{-6}$ M) ($CH_3CN/H_2O$, 5/5) with **5** and $Hg^{2+}$.

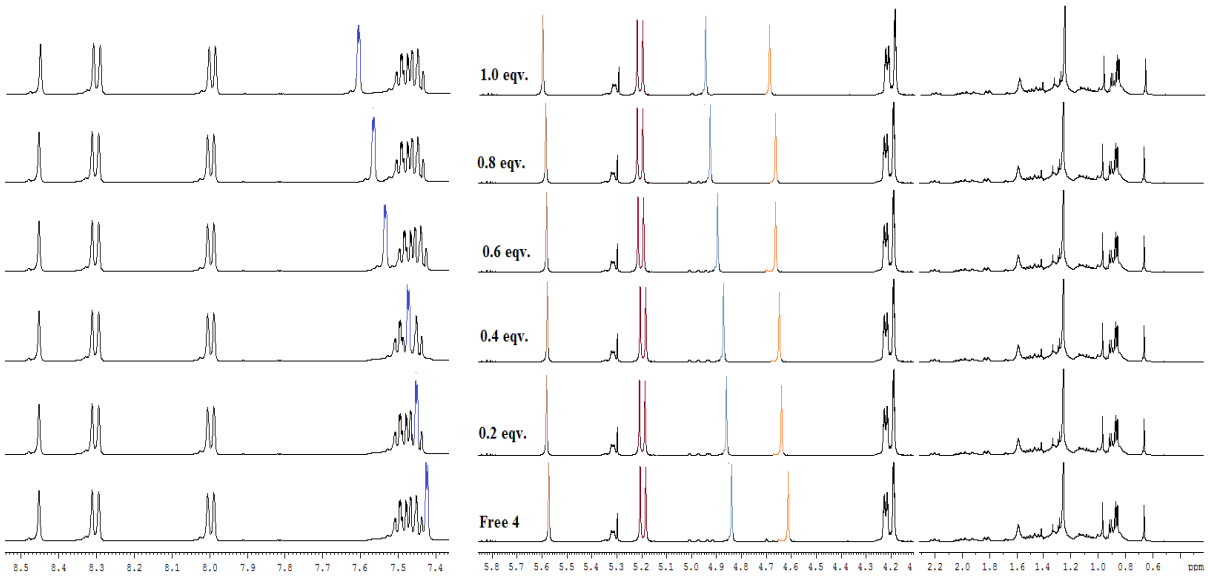



**Figure S17**. $^{1}$H NMR titration of **4** upon addition of increasing amount of $Hg^{2+}$ up to 1 equiv in $CD_3CN$ solution.

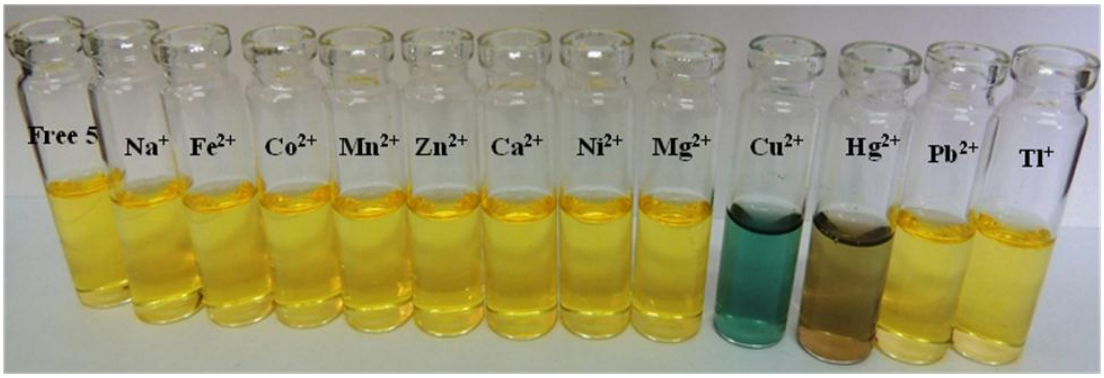



**Figure S18.** Evolution of the color in $CH_3CN$ solution of **5** ($10^{-5}$ M) after addition of 5 equiv of different cations tested as perchlorate salt.

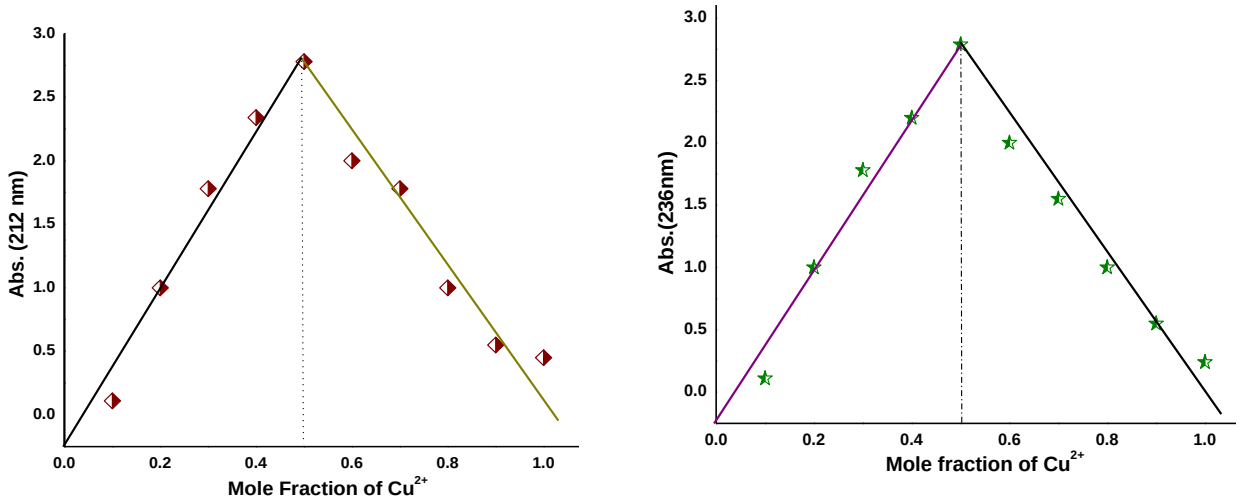



**Figure S19.** Job's plot for compounds **4** and **5** in presence of $Cu^{2+}$ ion.

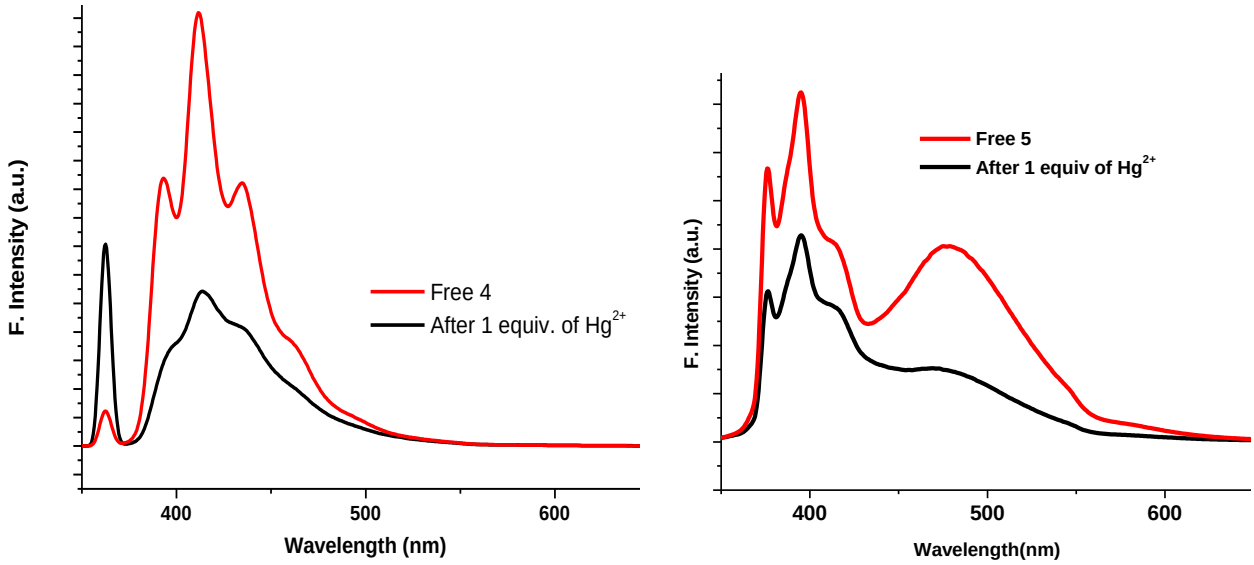



**Figure S20.** Fluorescene emission change of **4** (2 nM) at $\lambda_{exc}$ = 363 nm (top) and **5** (2nM) at $\lambda_{exc}$ = 345 nm (bottom) upon addition of $Hg^{2+}$ ion upto 1 equiv in $CH_3CN/H_2O$ (1/1).

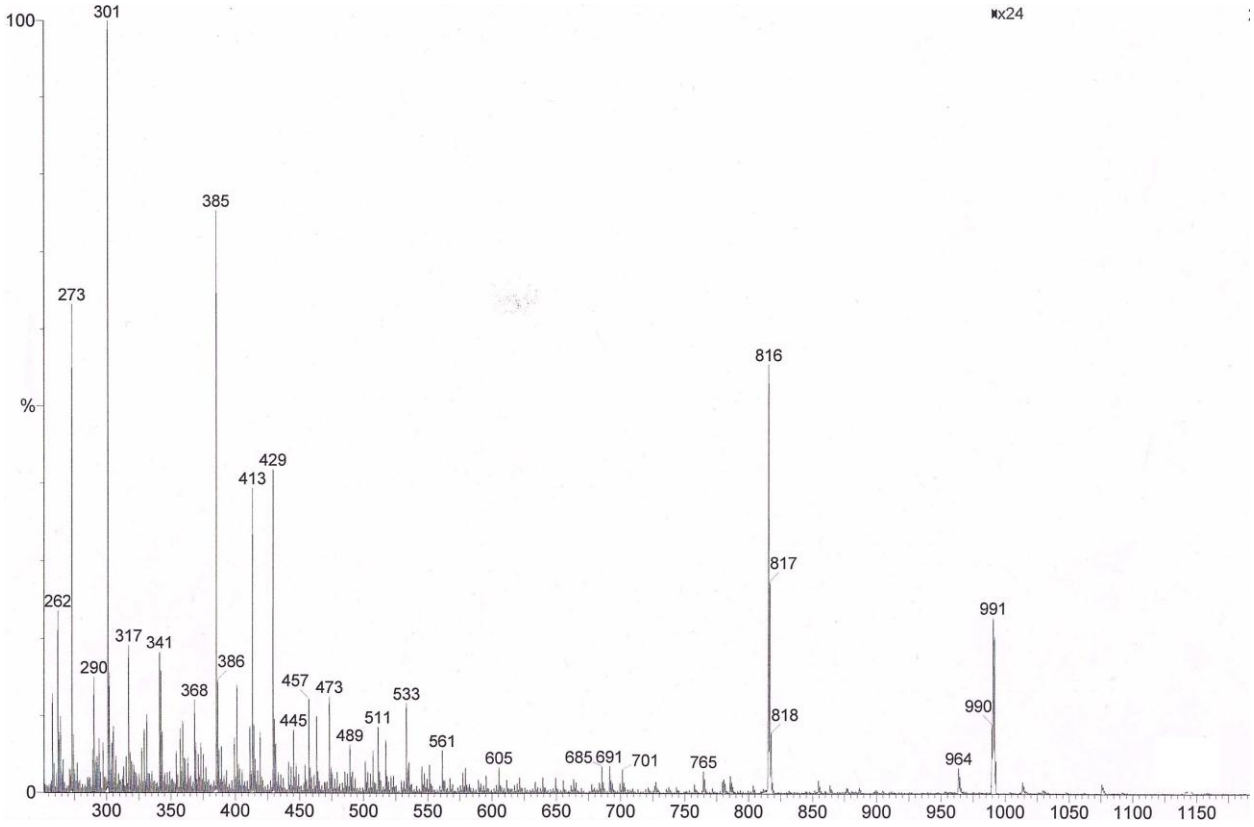



**Figure S21.** Electospray mass spectrum of **5.**