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Electronic Supporting Information

Cyclic *vs* Acyclic Alkyne towards Hg^{2+} ion detection: A Combined Experimental and Theoretical Studies

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Contents **Page**

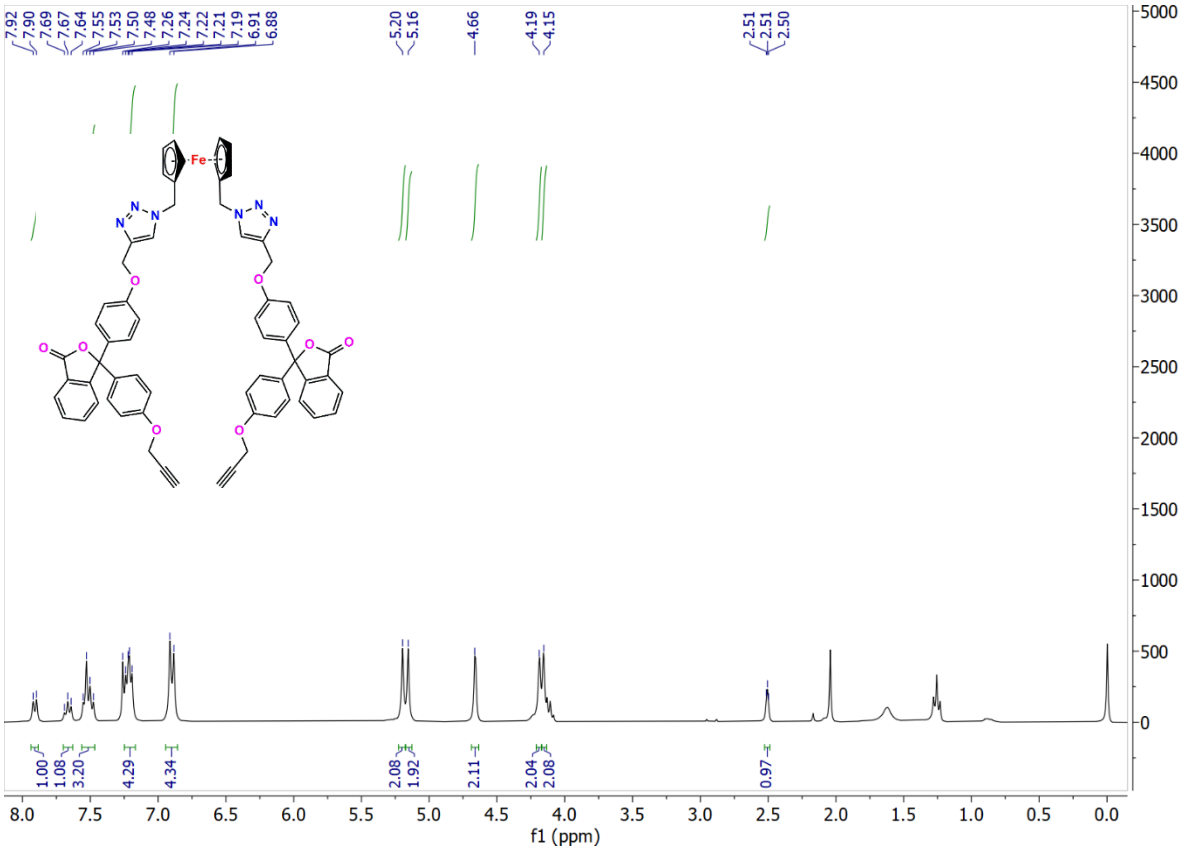

Fig. S1: ^{1}H NMR spectra of **3** in $CDCl_3$.

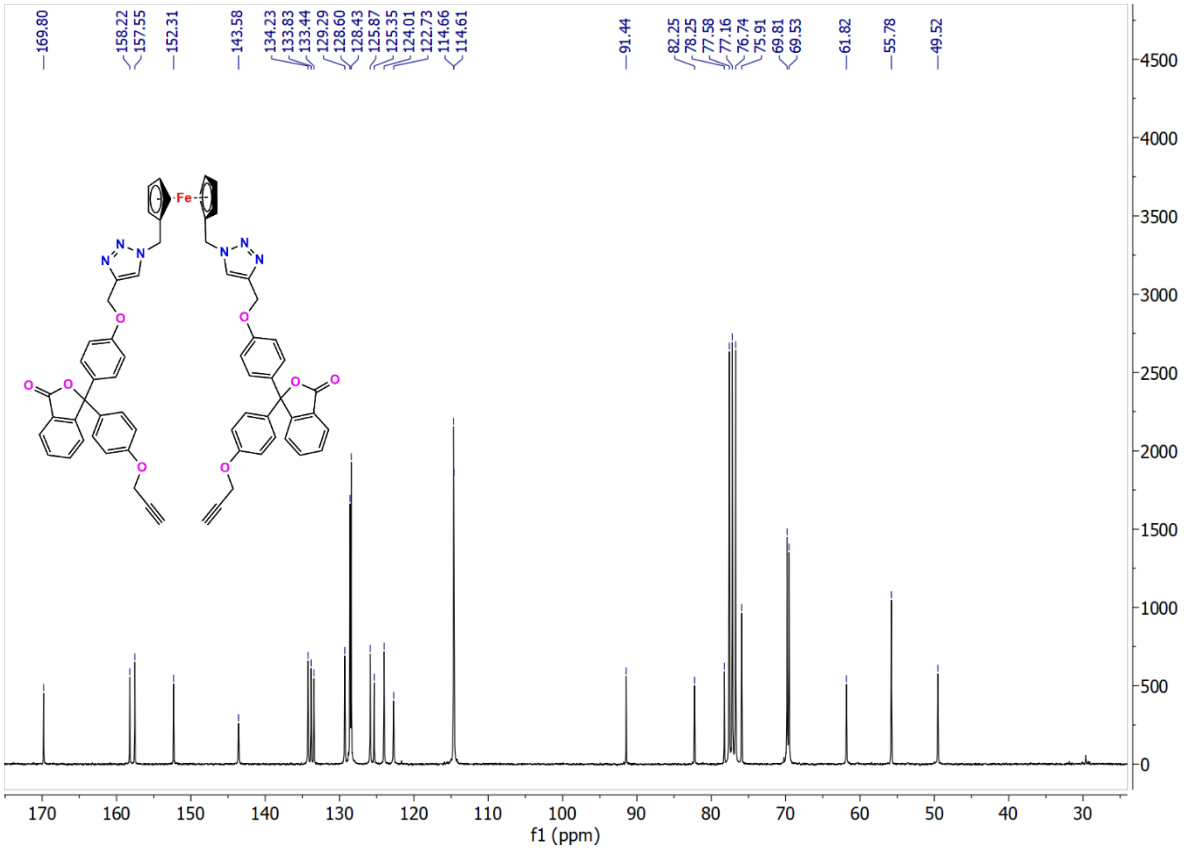

Fig. S2: ^{13}C NMR spectra of **3** in $CDCl_3$.

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
5123 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Fe
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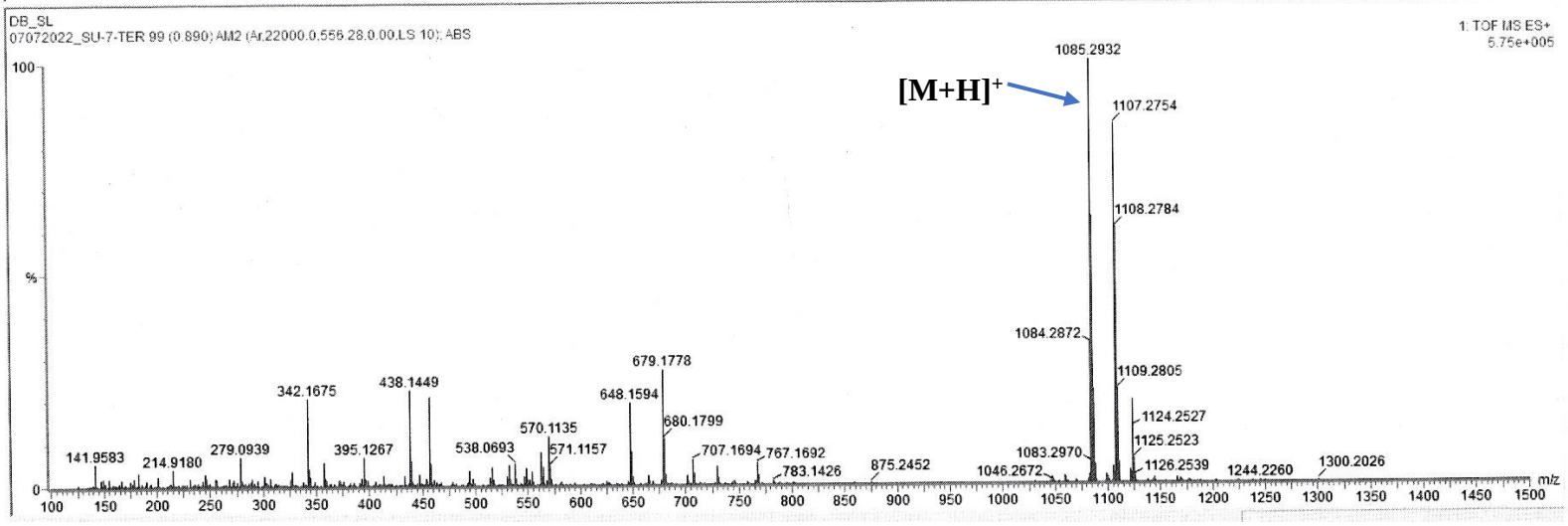


Fig. S3: HRMS of **3**.

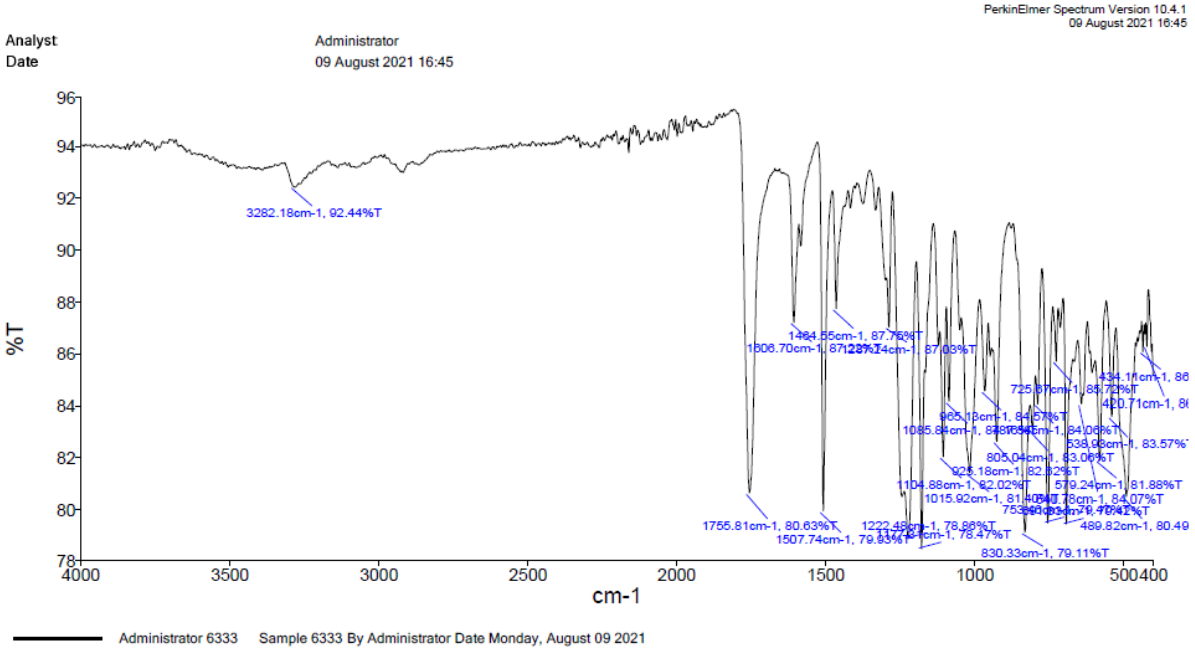


Fig. S4: IR spectrum of **3**.

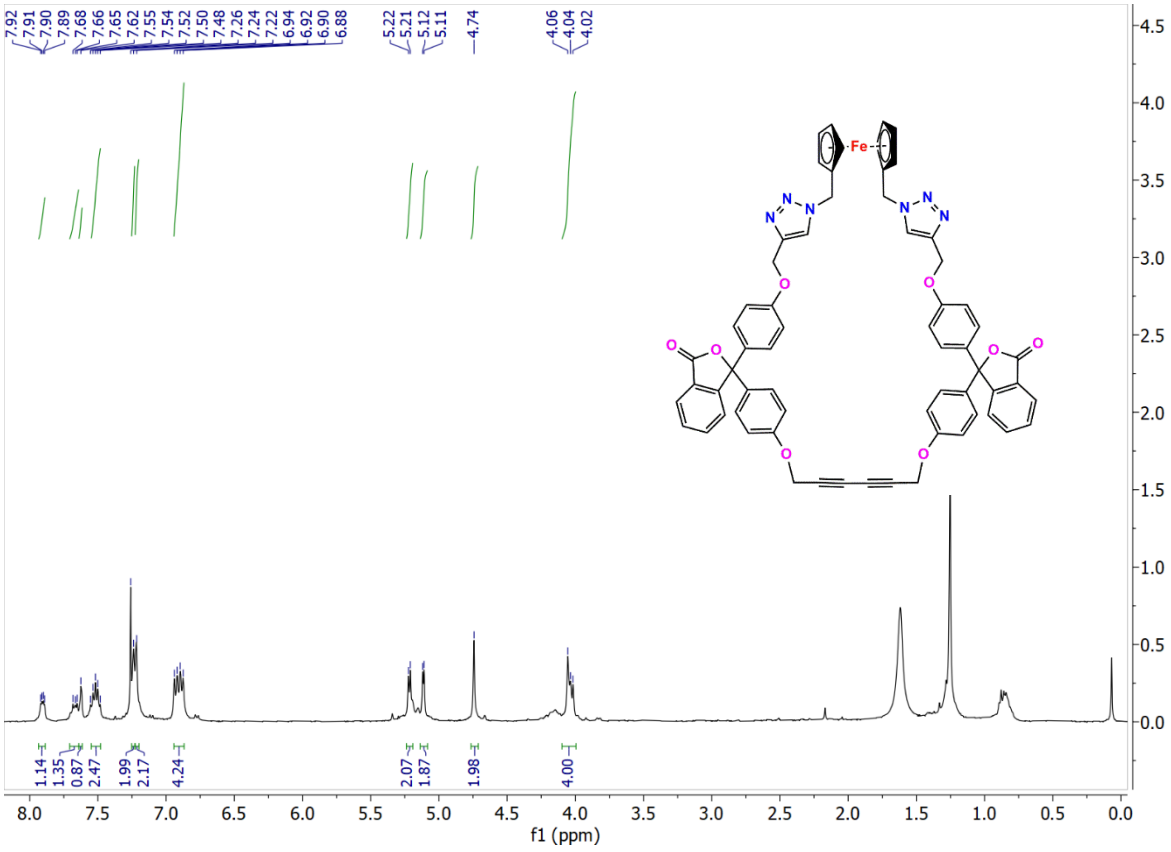


Fig. S5: ^{1}H NMR spectra of **4** in $CDCl_3$.

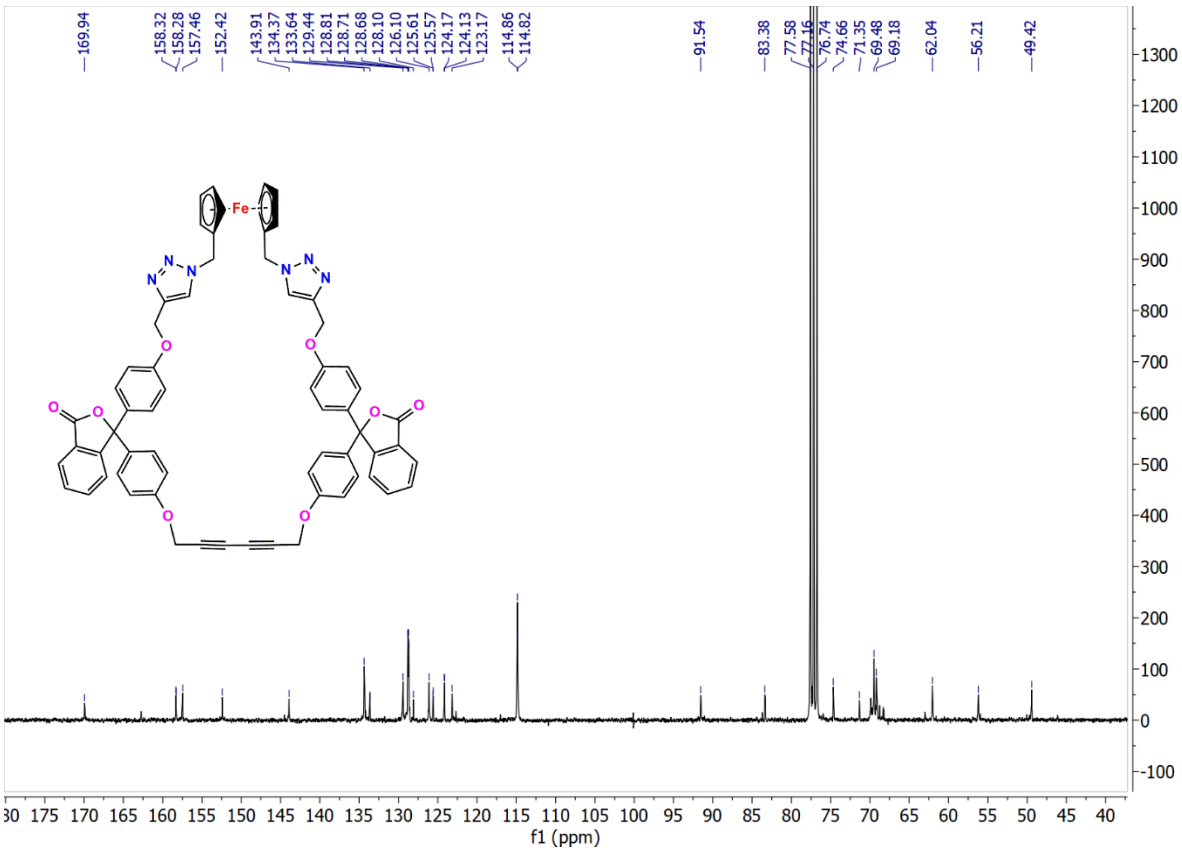


Fig. S6: ^{13}C NMR spectra of **4** in $CDCl_3$.

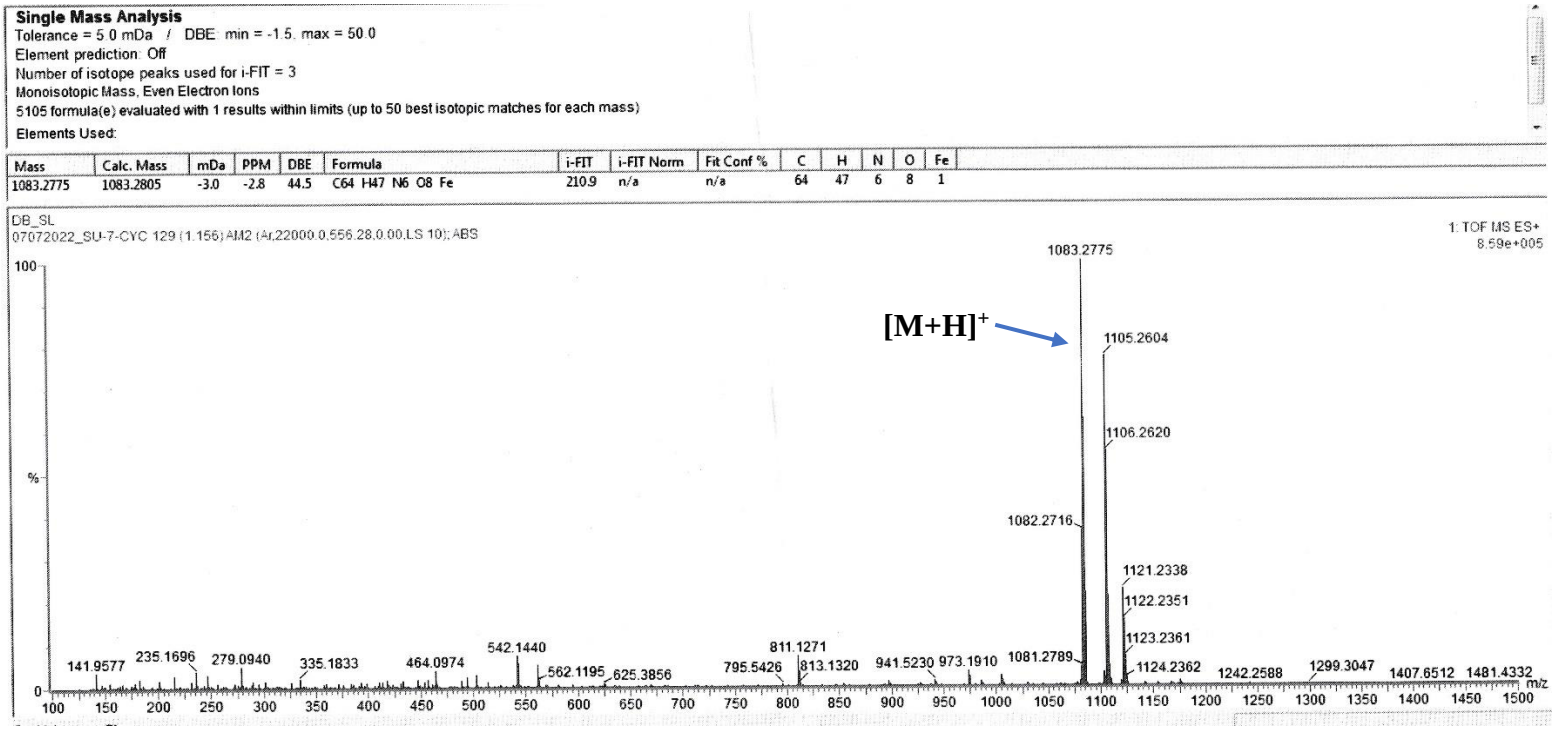


Fig. S7: HRMS of **4**.

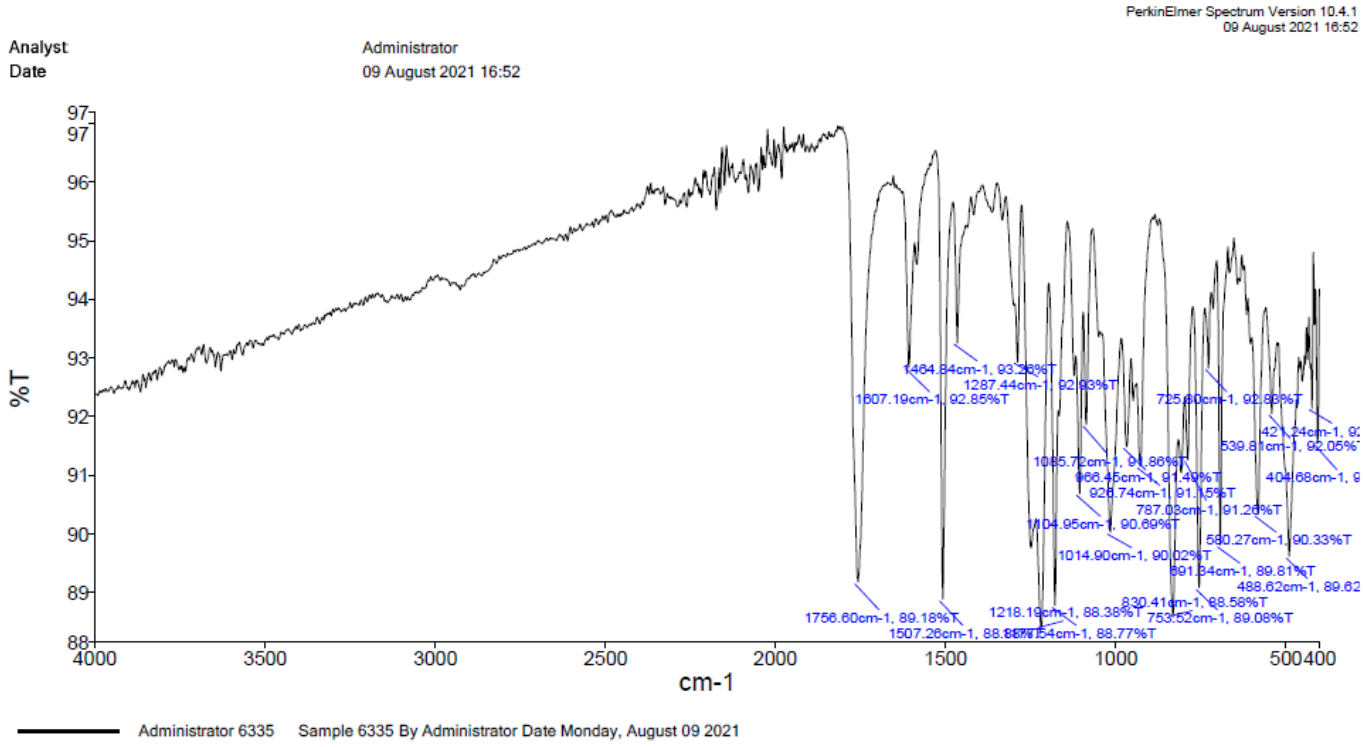


Fig. S8: IR spectrum of **4**.

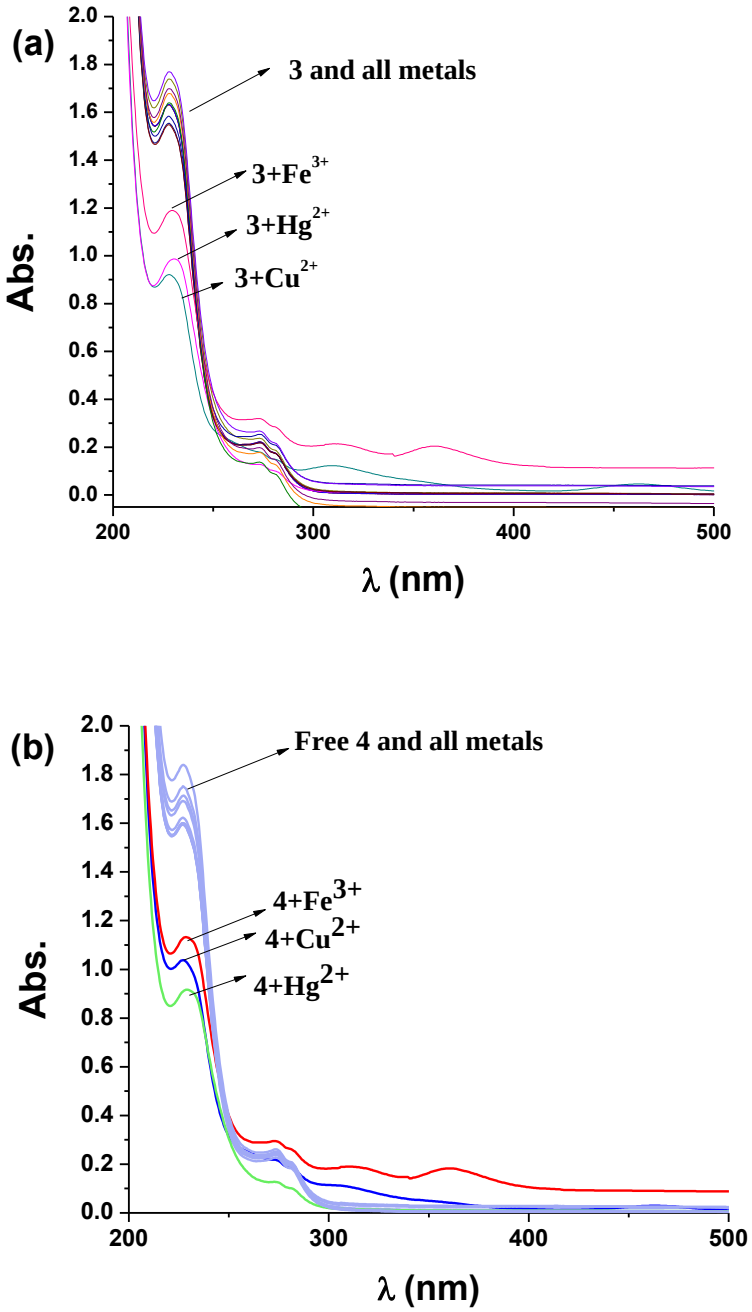


Fig. S9: UV-vis titrations of compounds (a) **3** and (b) **4** in presence of several metal ions (CH_3CN, 3.12×10^{-5} M).

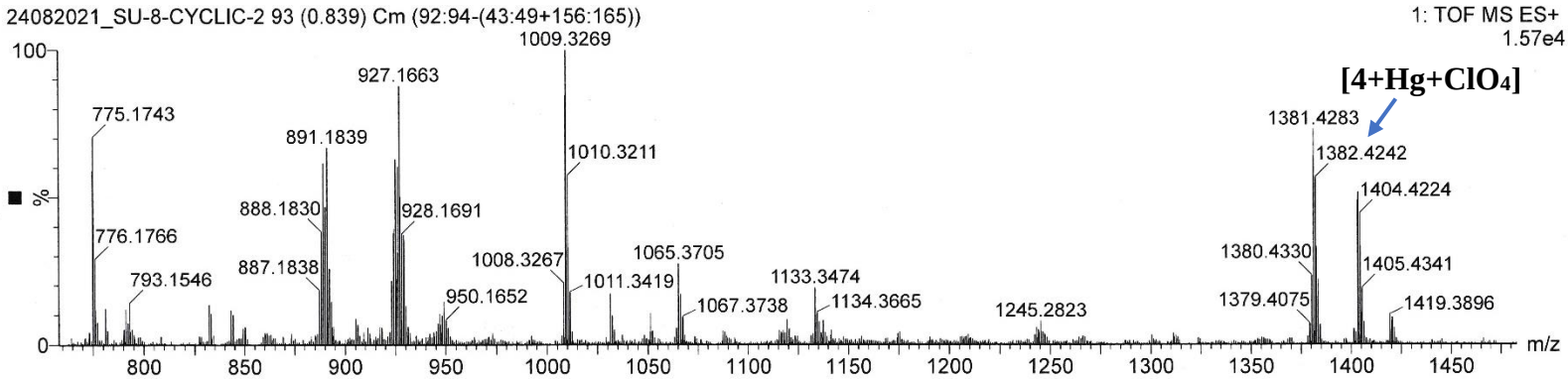


Fig. S10: HRMS of [**4**+Hg+ClO_4].

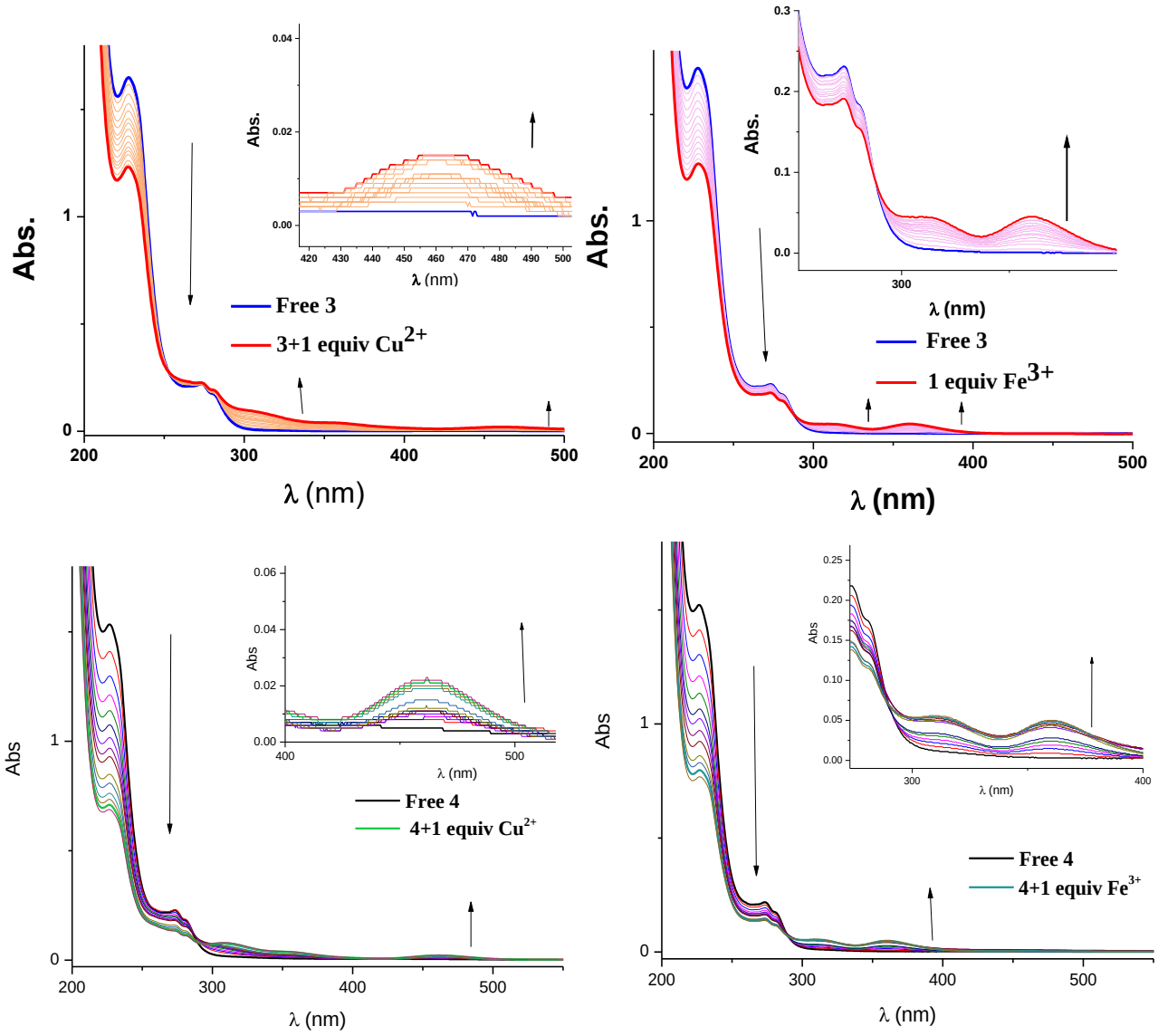


Fig. S11: UV-vis titrations of compounds **3** (CH_3CN, 3.12×10^{-5} M) and **4** (CH_3CN, 3.12×10^{-5} M) in presence of up to 1 equiv Cu^{2+} and Fe^{3+} ions (CH_3CN, 3.12×10^{-5} M).

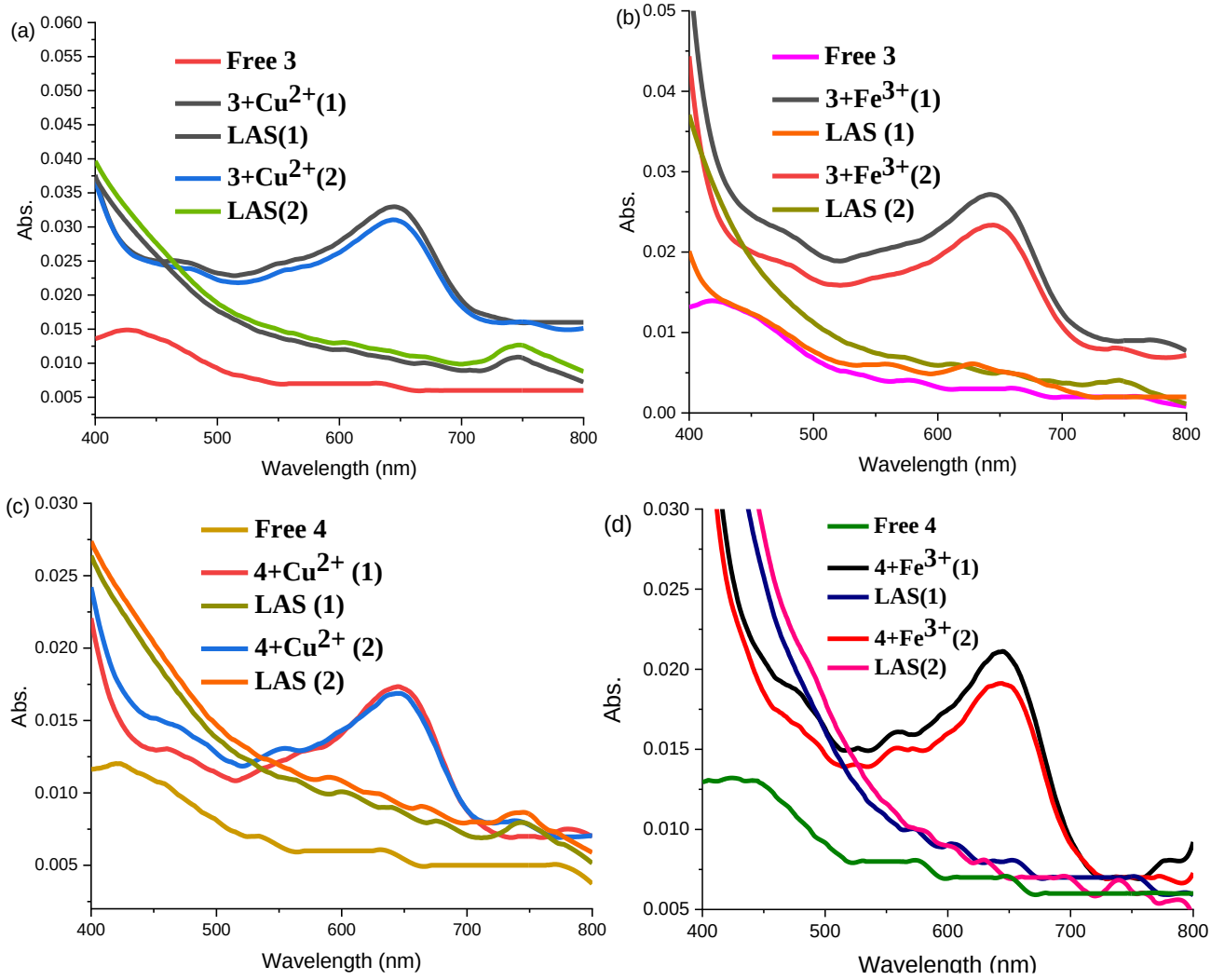


Fig. S12: Reversible oxidation-reduction interaction studies using UV-vis spectroscopic analysis of ferrocene centers of compounds **3** (CH_3CN, 3.12×10^{-5} M) and **4** (CH_3CN, 3.12×10^{-5} M) in presence of up to 1 equiv Cu^{2+}/Fe^{3+} ions (CH_3CN, 1×10^{-3} M) (oxidant) and Sodium-L-ascorbate (LAS) (H_2O, 1×10^{-3} M) (reductant) alternatively.

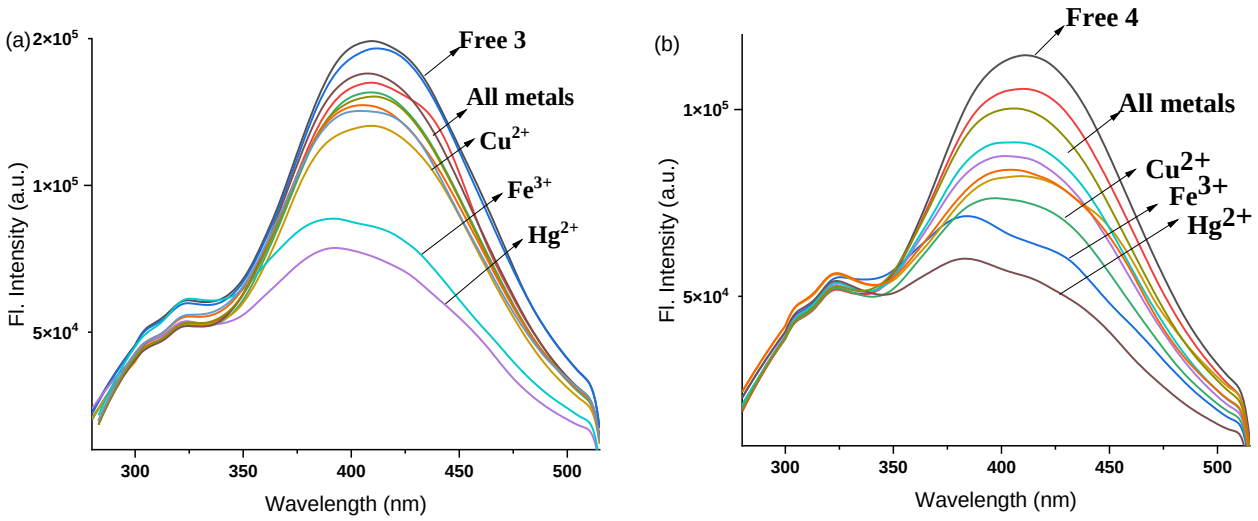
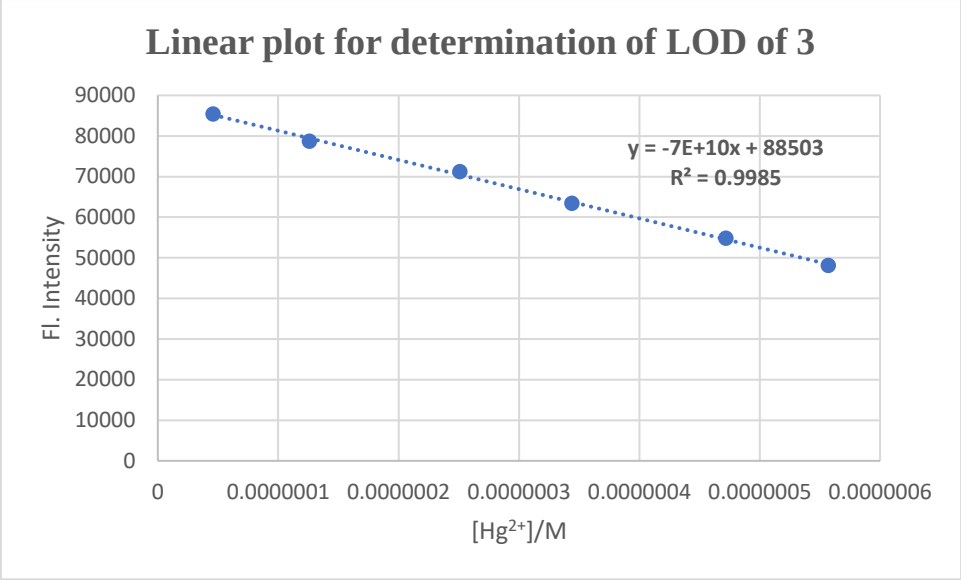


Fig. S13: Fluorescence spectra of compounds (a) **3** (CH_3CN, 9.7×10^{-7} M) and (b) **4** (CH_3CN, 9.7×10^{-7} M) in presence of several metal ions (CH_3CN, 9.7×10^{-7} M).

(a)



(b)

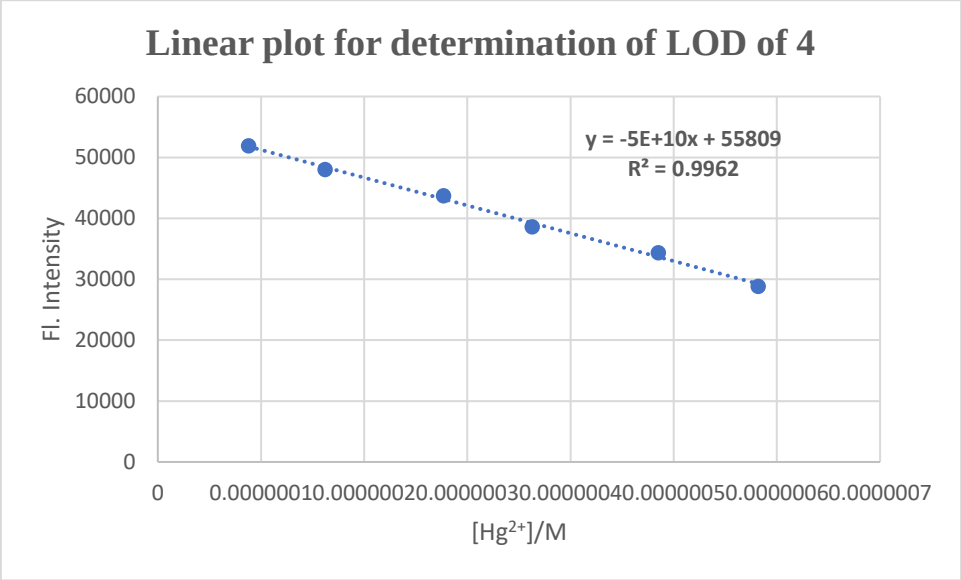


Fig. S14: Linear plots for the determination of LOD for (a) **3** and (b) **4** from fluorescence experiments.

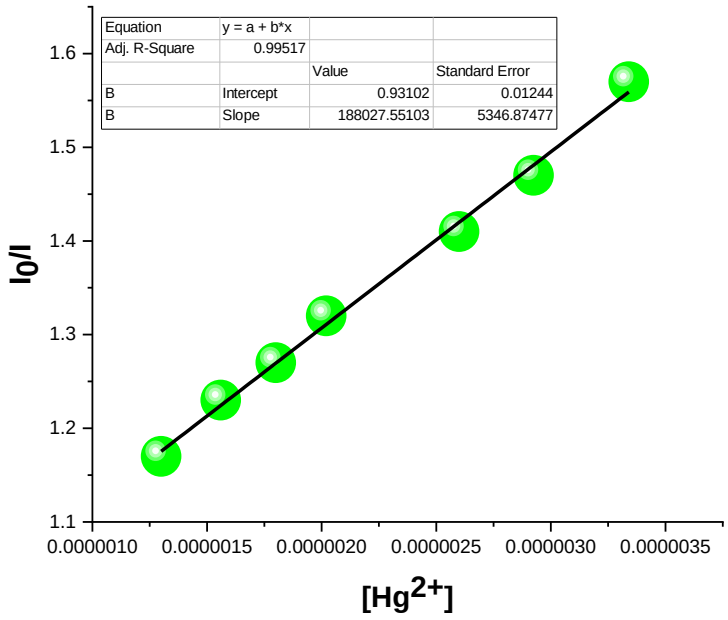
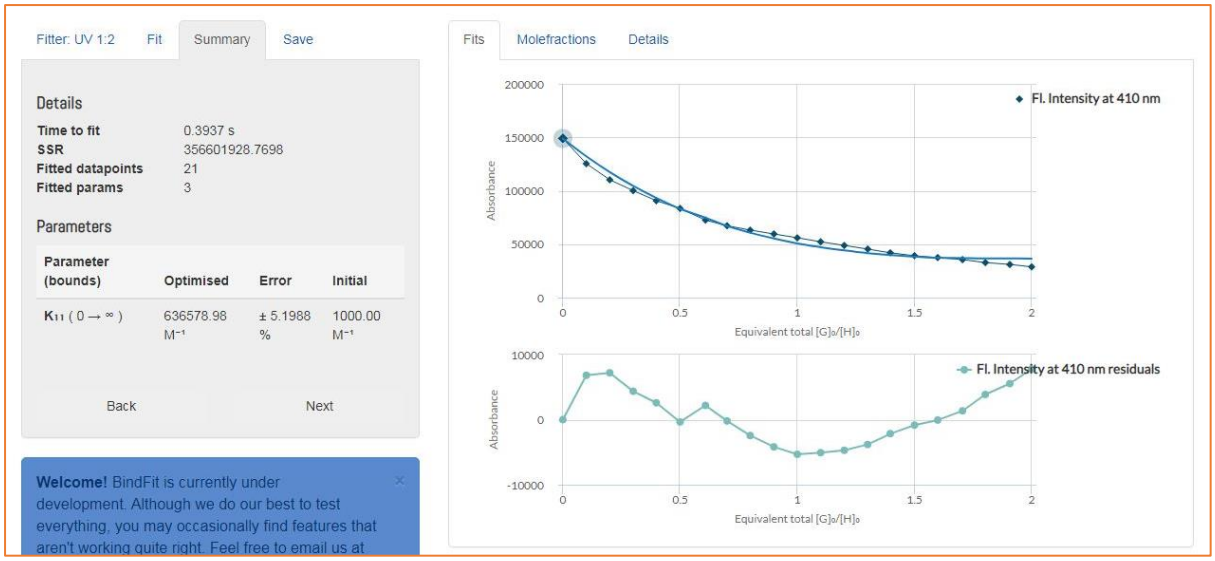


Fig. S15: Binding constant of compound **4** by using Stern-Volmer equation from fluorescence titration in presence of Hg^{2+}.

(a)



(b)

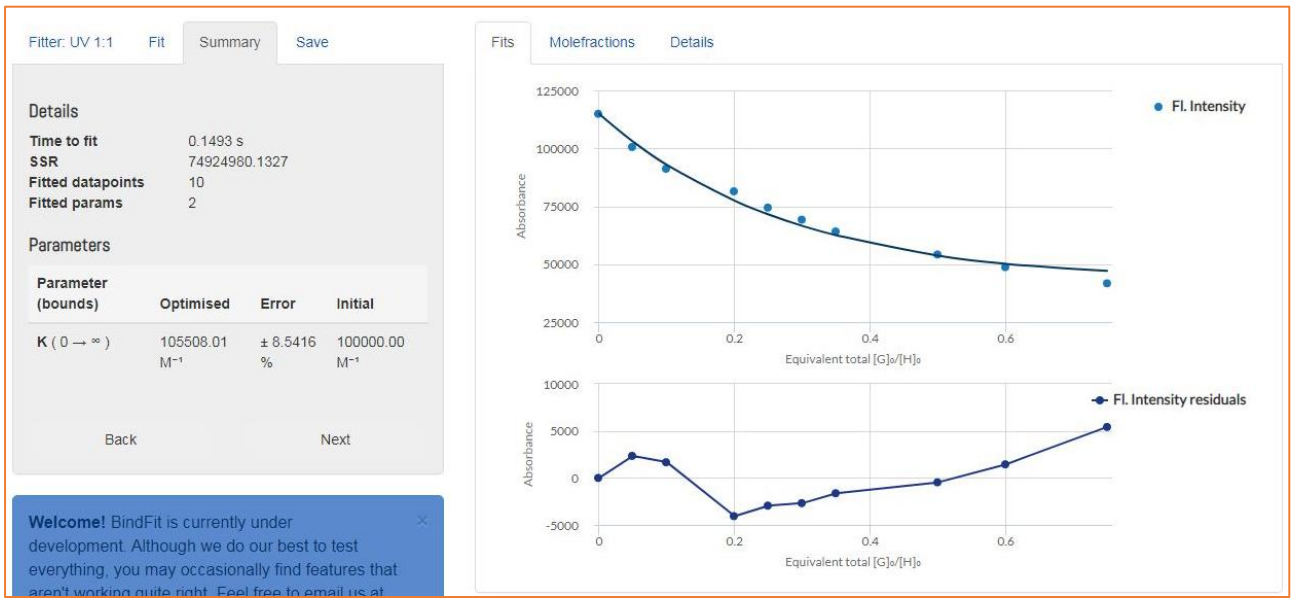


Fig. S16: Bindfit plots for Hg^{2+}-binding by (a) **3** in 1:2 (non-cooperative) stoichiometry and (b) **4** in 1:1 stoichiometry from fluorescence titration using L-BFGS-B fit. Screenshots taken from the website supramolecular.org.

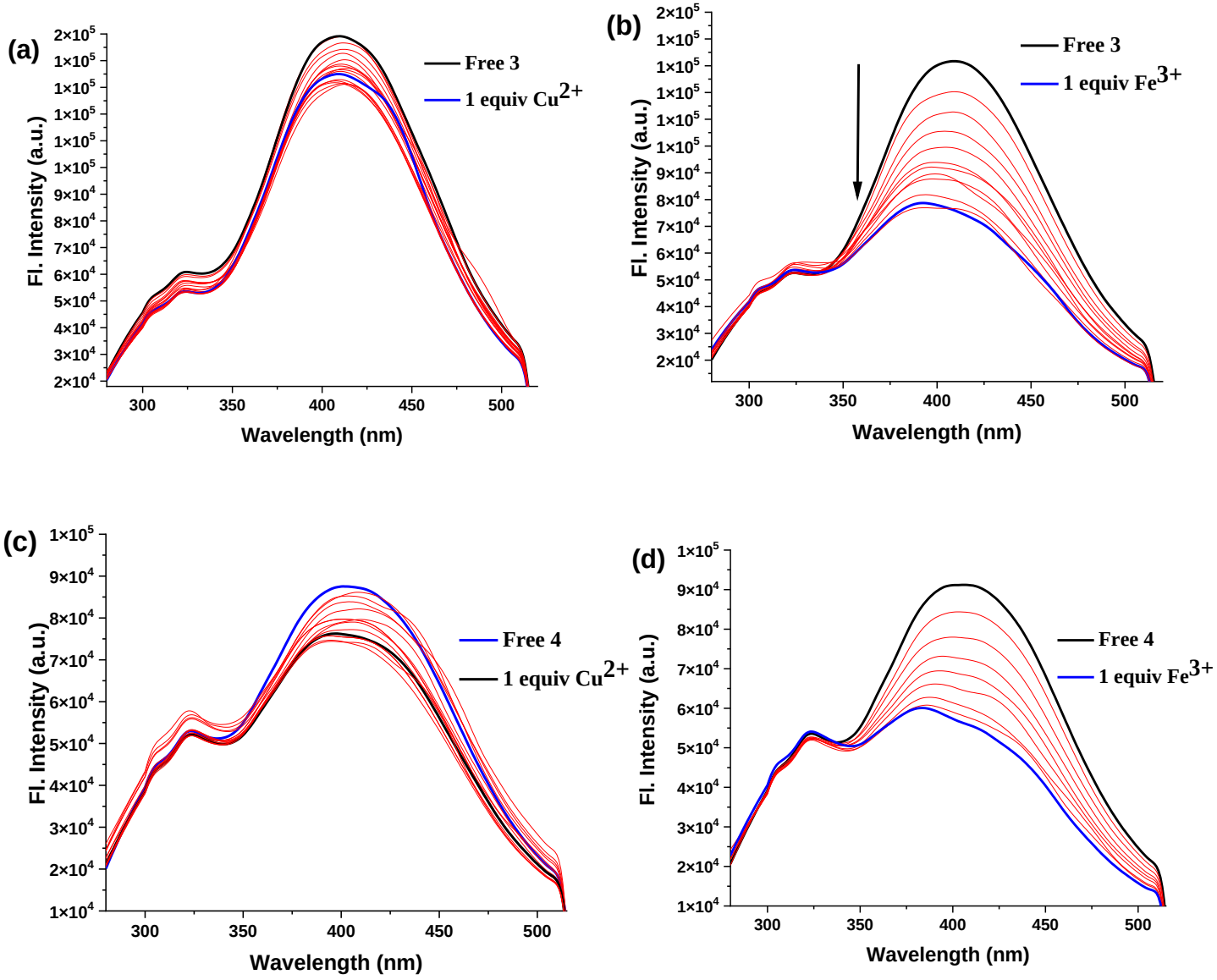


Fig. S17: Fluorescence titrations of compounds (a), (b) **3** (CH_3CN, 9.7×10^{-7} M) and (c), (d) **4** (CH_3CN, 9.7×10^{-7} M) in presence of up to 1 equiv Cu^{2+} and Fe^{3+} ions (CH_3CN, 9.7×10^{-7} M).

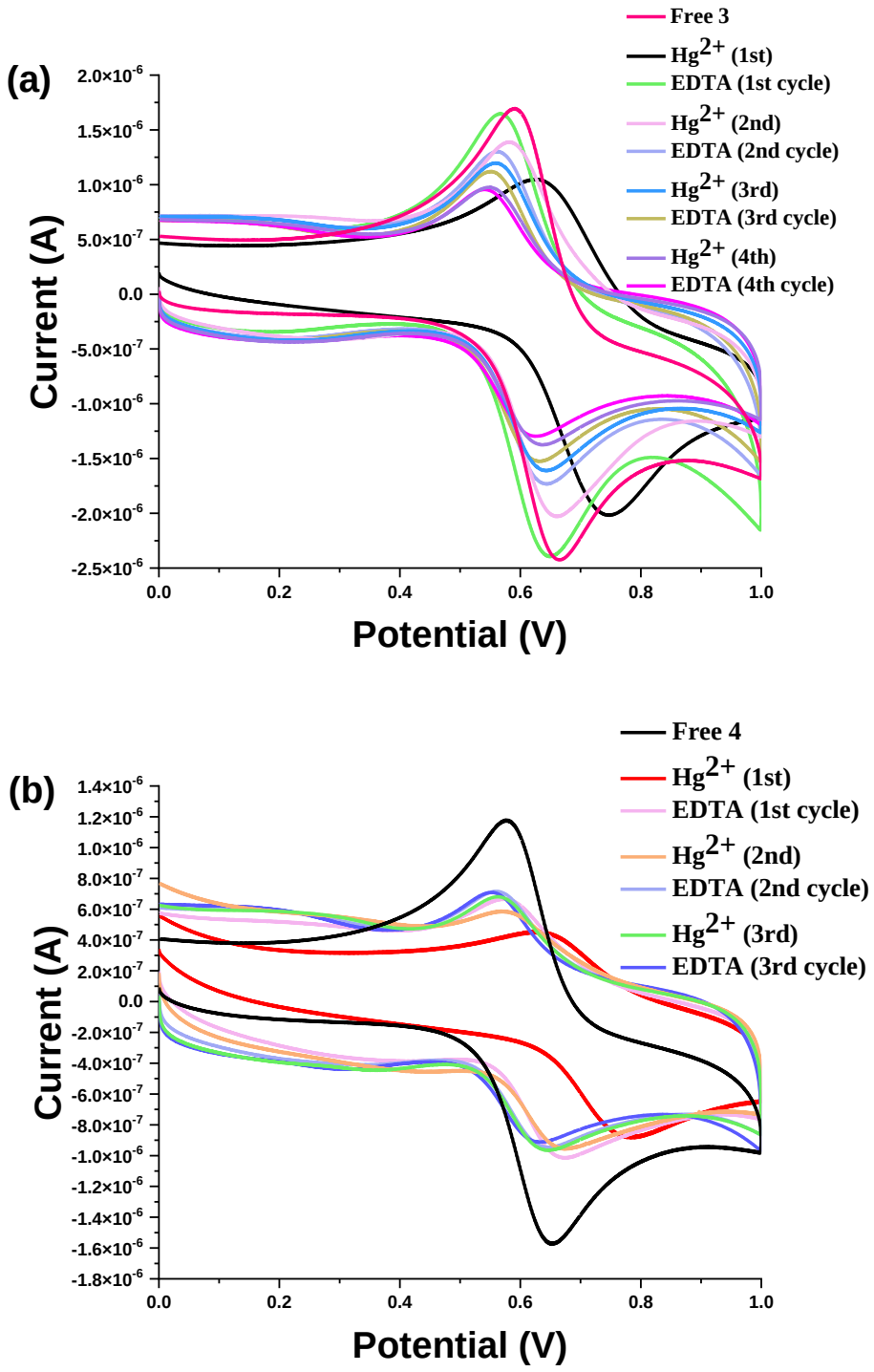


Fig. S18: Reversibility of the interactions of compounds (a) **3** (CH_3CN, 2.5 × 10^{-4} M) and (b) **4** (CH_3CN, 2.5 × 10^{-4} M) with Hg^{2+} (CH_3CN, 2.5 × 10^{-4} M) tested by employing aqueous solution of Na_2EDTA (H_2O, 2.5 × 10^{-4} M).

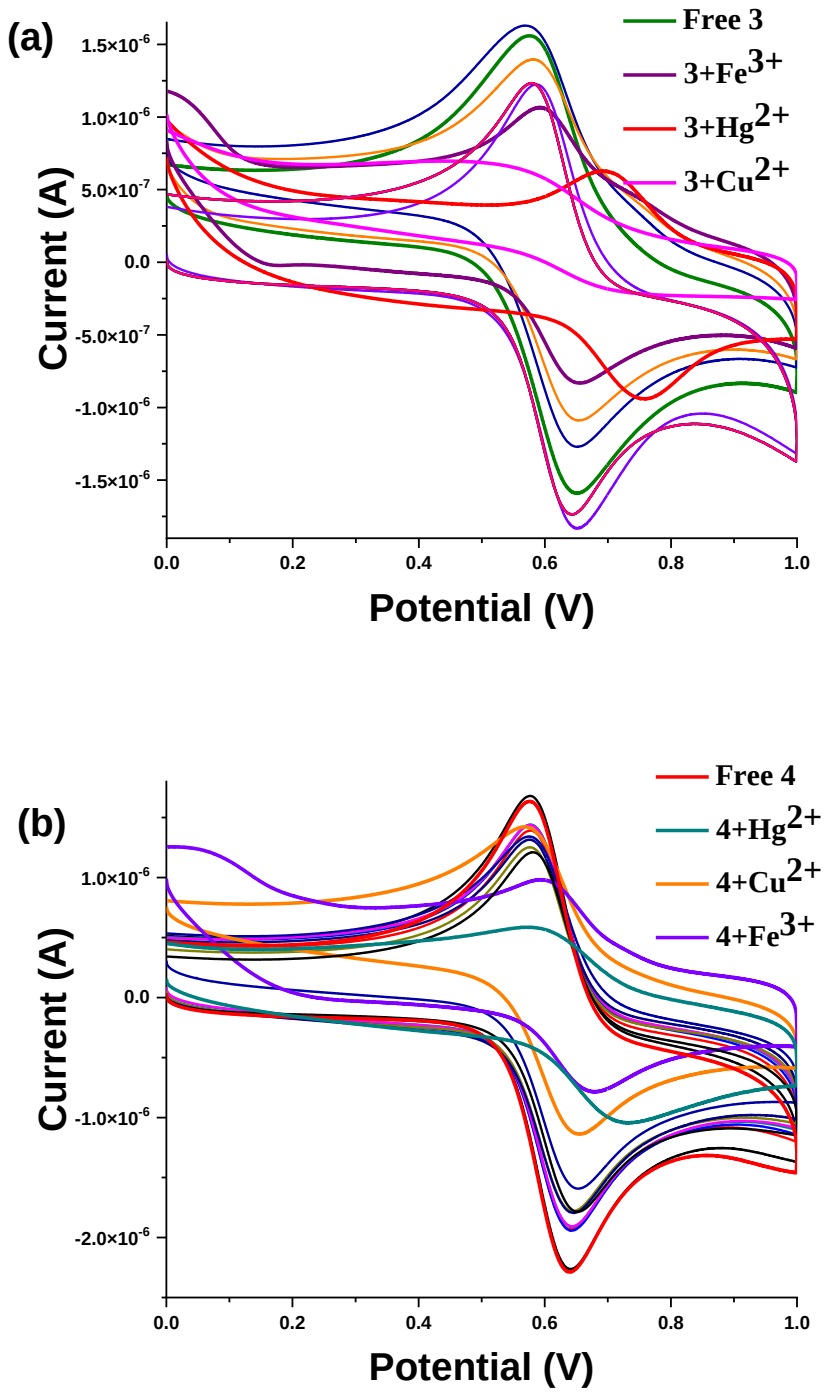


Fig. S19: CV of compounds (a) **3** (CH_3CN, 2.5×10^{-4} M) and (b) **4** (CH_3CN, 2.5×10^{-4} M) in presence of all metal ions (CH_3CN, 2.5×10^{-4} M) under scan rate 0.06 Vs^{-1}.

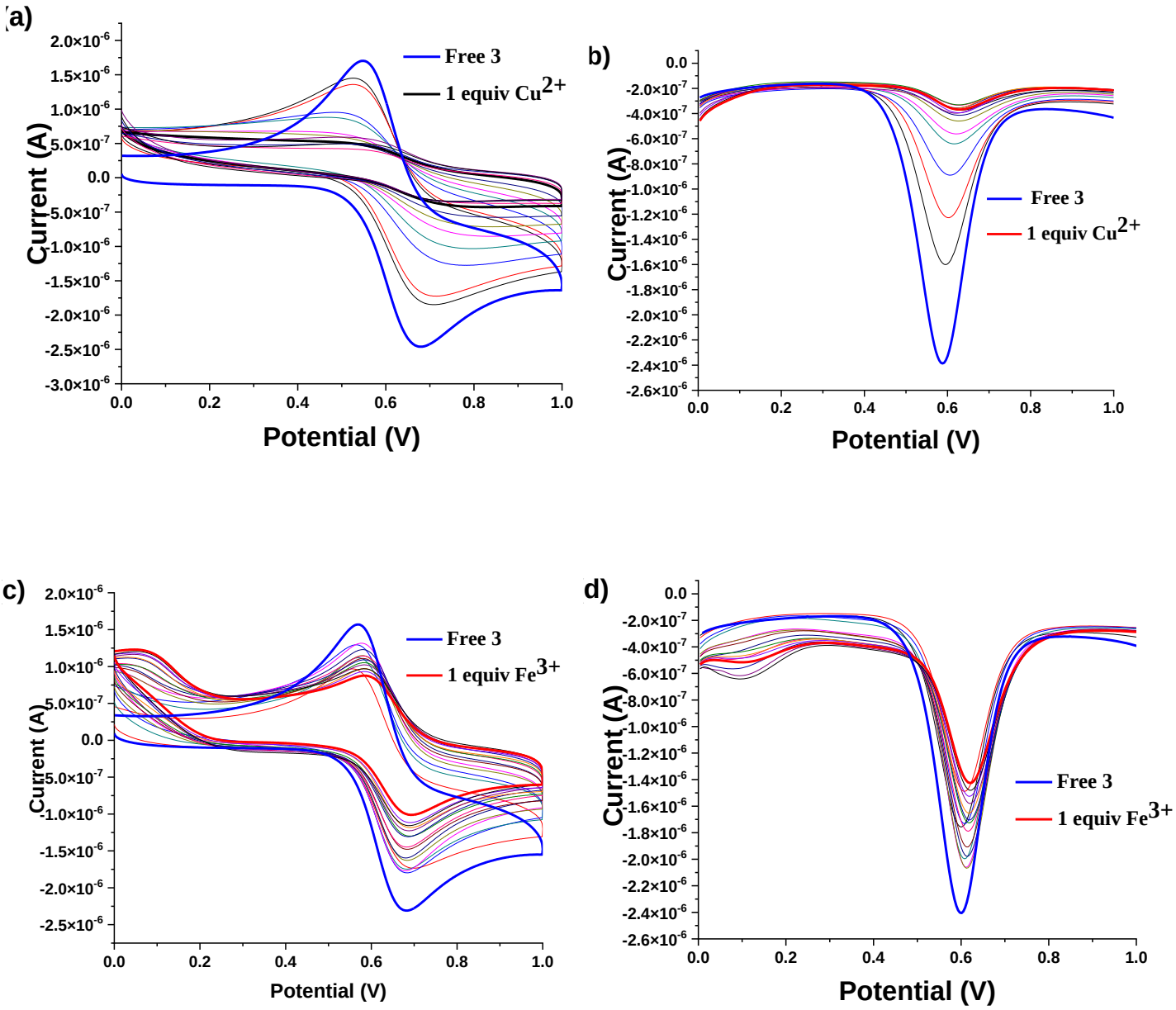


Fig. S20: CV and DPV of compound **3** (CH_3CN, 2.5 × 10^{-4} M) in presence of up to (a), (b) 1 equiv Cu^{2+} (CH_3CN, 2.5 × 10^{-4} M) and (c), (d) Fe^{3+} ions (CH_3CN, 2.5 × 10^{-4} M) under scan rate 0.06 Vs^{-1}.

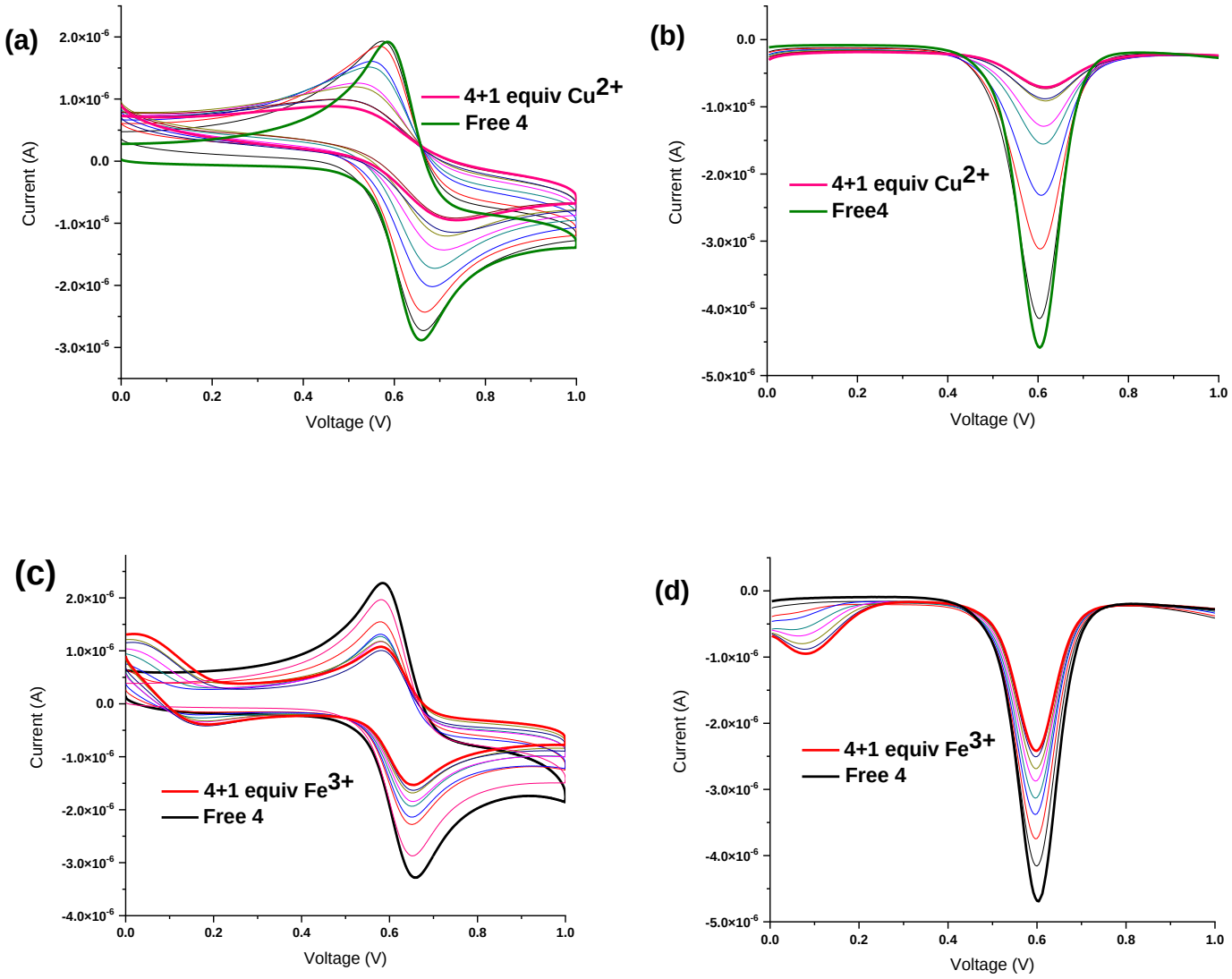


Fig. S21: CV and DPV of compound **4** (CH_3CN, 2.5 × 10^{-4} M) in presence of up to 1 equiv Cu^{2+} (CH_3CN, 2.5 × 10^{-4} M) and Fe^{3+} ions (CH_3CN, 2.5 × 10^{-4} M) under scan rate 0.06 Vs^{-1}.

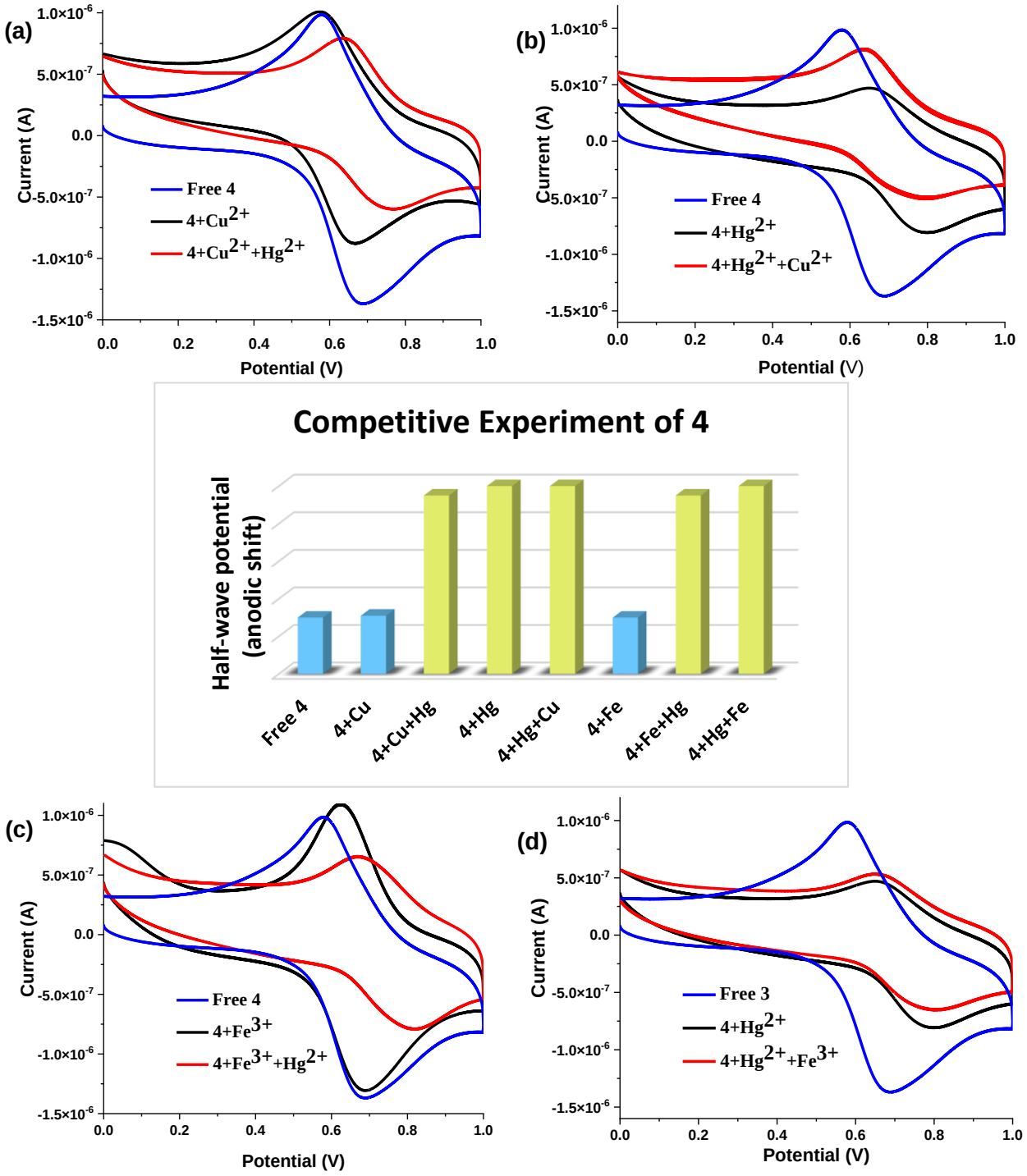


Fig. S22: Competition experiment of compound **4** (CH_3CN, 2.5×10^{-4} M) with (a), (b) Cu^{2+}/Hg^{2+} couple (CH_3CN, 2.5×10^{-4} M) and (c), (d) Fe^{3+}/Hg^{2+} couple (CH_3CN, 2.5×10^{-4} M) under scan rate 0.06 Vs^{-1}.

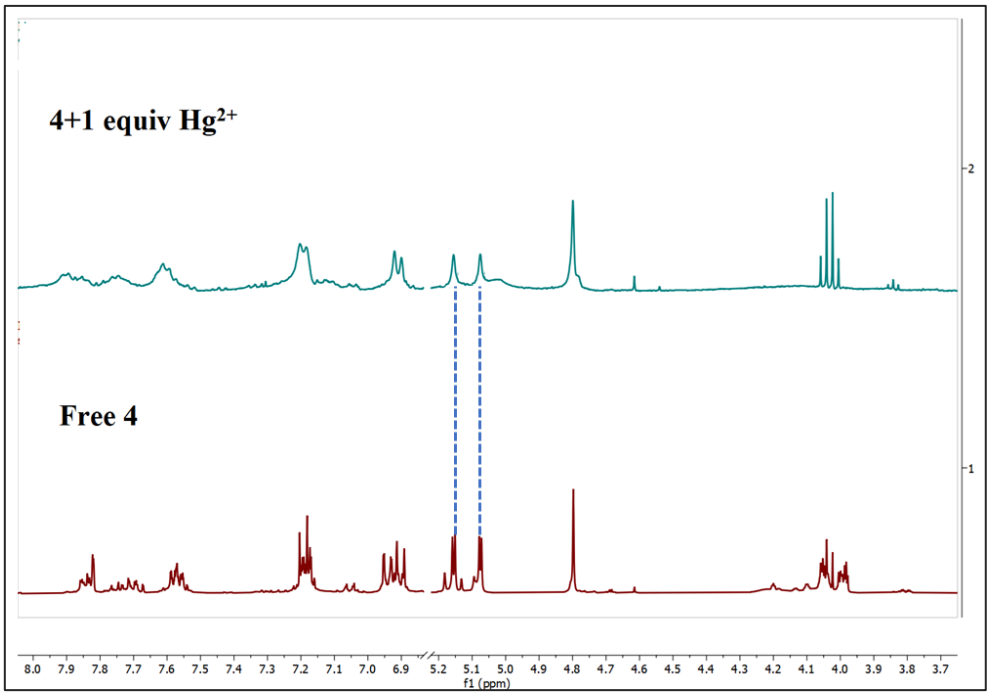
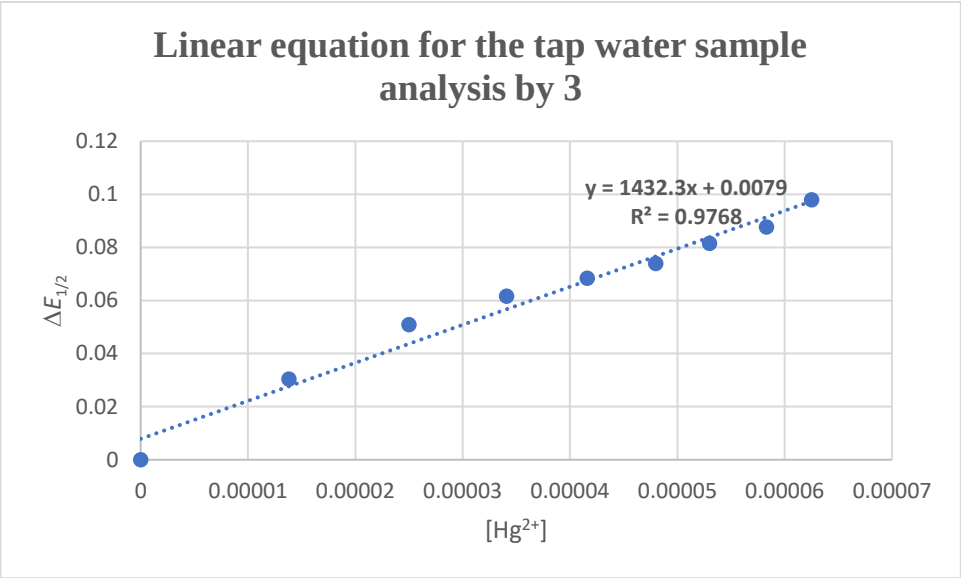


Fig. S23. ^{1}H NMR of compound **4** before and after addition of 1 equiv of Hg^{2+} ion in CD_3CN.

Fig. S24. Colorimetric test of (a) compound **3** (1×10^{-3} M CH_3CN) and (b) compound **4** (1×10^{-3} M CH_3CN) in presence of several metal ions (1×10^{-4} M CH_3CN) at neutral pH.

(a)



(b)

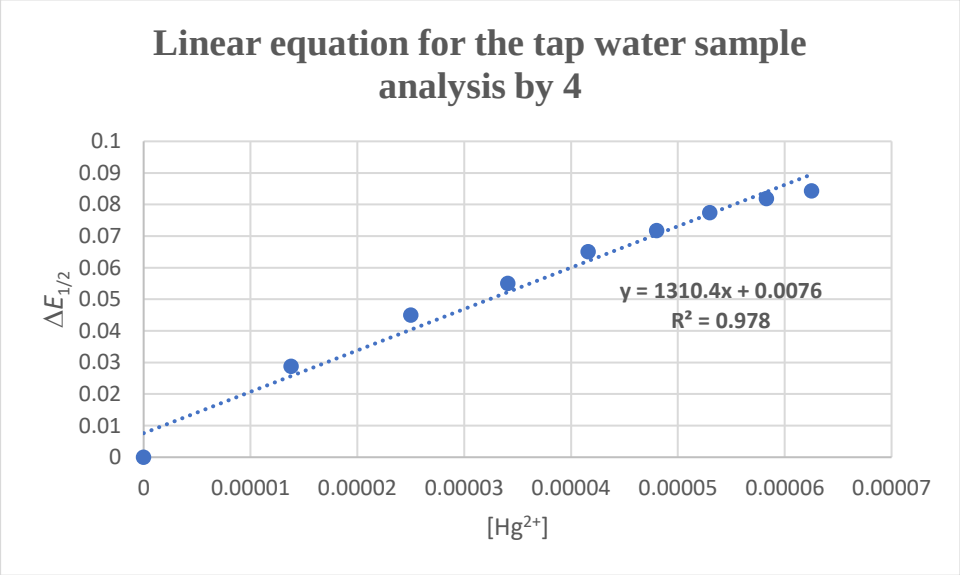
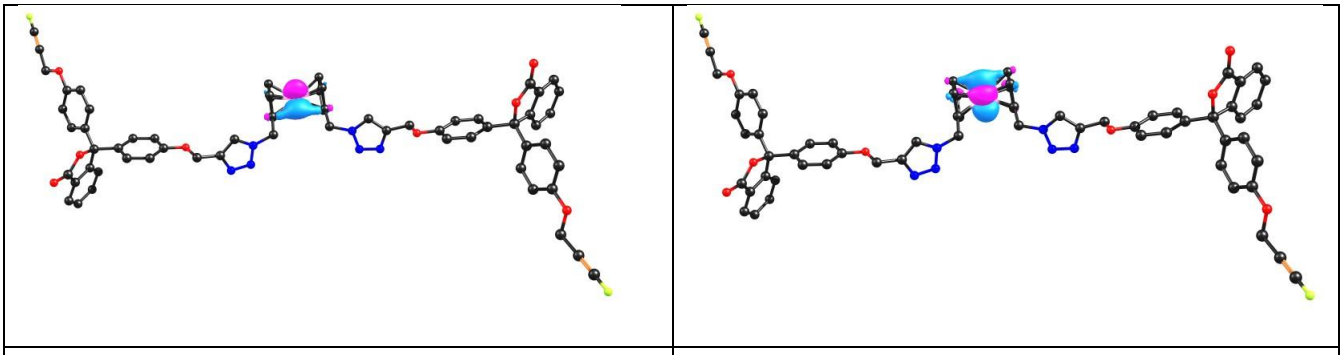
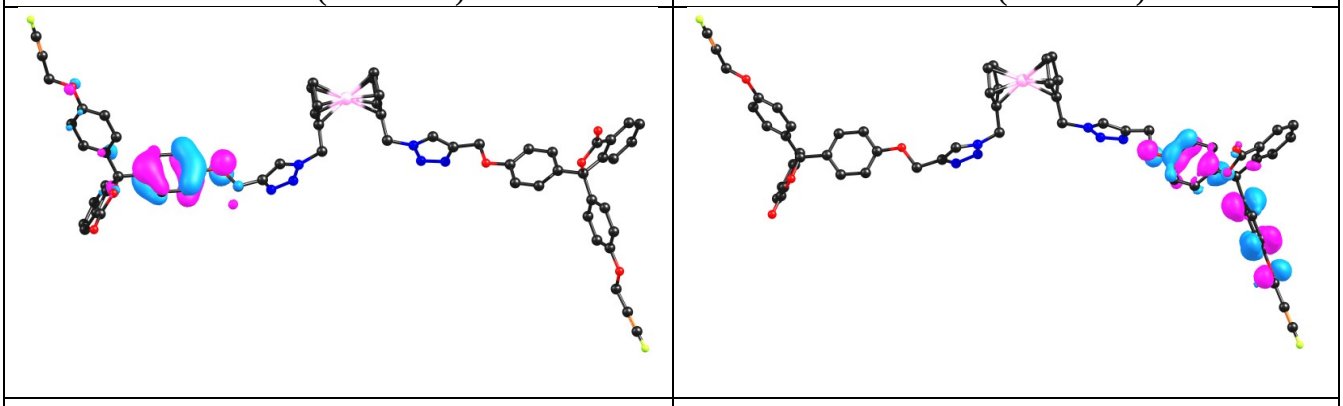


Fig. S25: Real sample analysis of tap water samples for the determination of Hg^{2+} ion by probes (a) **3** and (b) **4**.



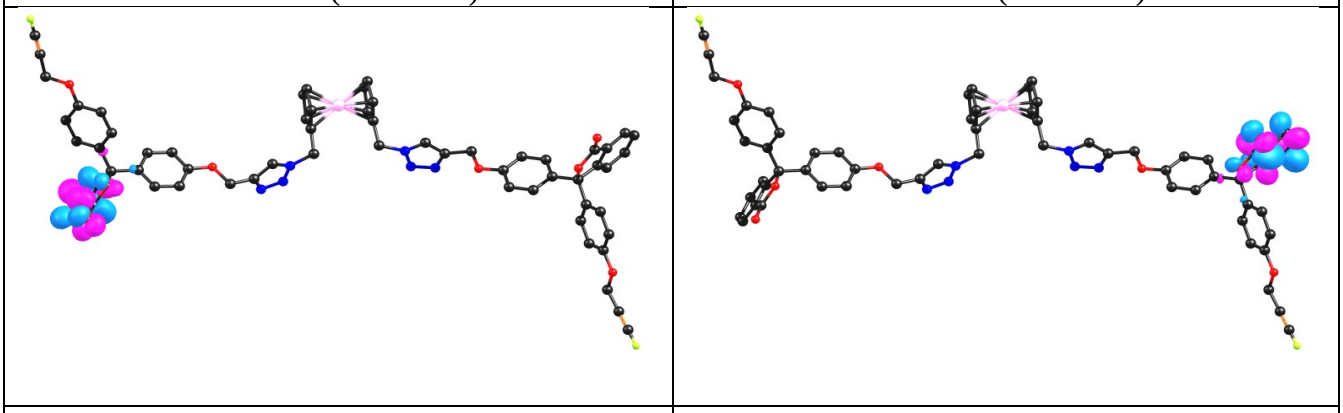
HOMO (**-5.934 eV**)

HOMO-1 (**-5.938 eV**)



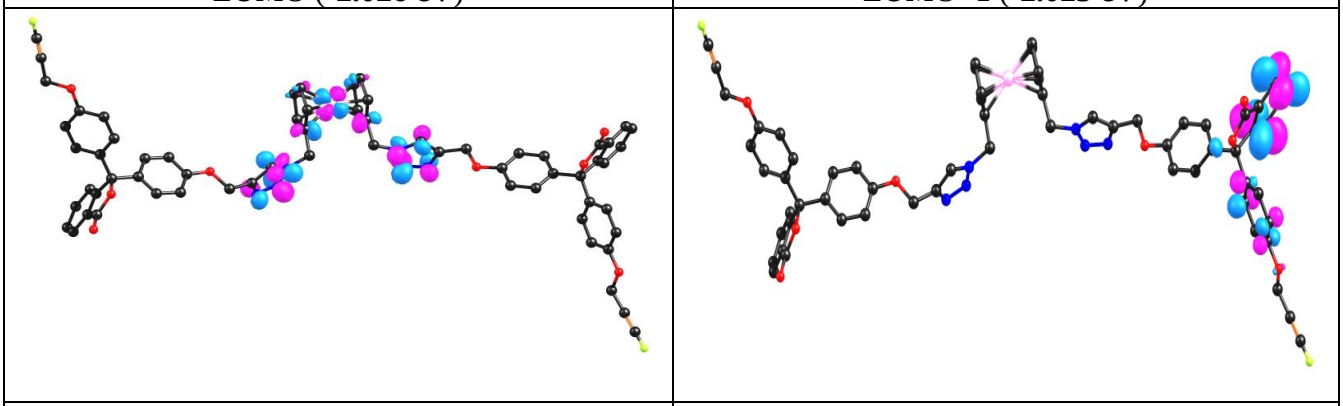
HOMO-2 (**-6.394** eV)

HOMO-3 (**-6.447 eV**)



LUMO (**-2.026 eV**)

LUMO+1 (**-2.025 eV**)



LUMO+2 (**-1.113** eV)

LUMO+3 (**-1.669** eV)

Fig. S26: Frontiers MOs of the acyclic ligand **3** with energy at B3LYP/ lanl2dz / CPCM (acetonitrile) level. (iso value= 0.04)

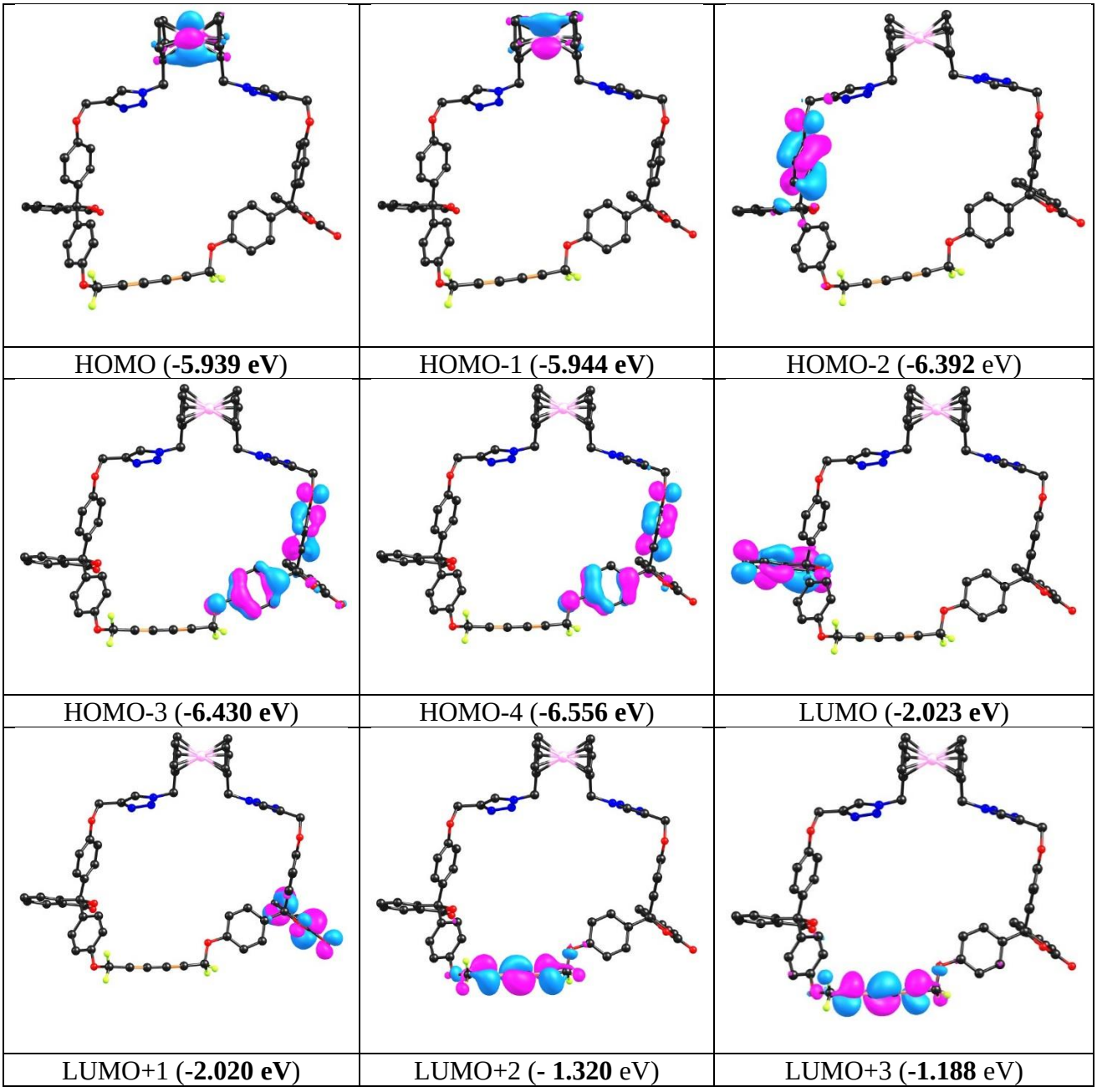
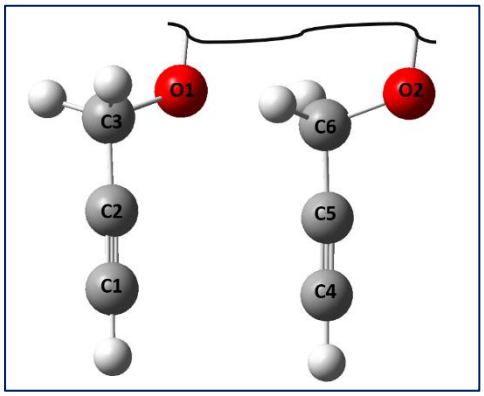


Fig. S27: Frontiers MOs of the cyclic ligand **4** with energy at B3LYP/ lanl2dz / CPCM (acetonitrile) level. (iso value=0.04)

Table S1. The selected distances (Å) and Wiberg Bond Index (WBI) of ligand/receptor **3** and **4** (involving only terminal alkynes as a binding unit) calculated at B3LYP/lanl2dz/cpcm (acetonitrile) level (The zoomed portions of the primary binding core of **3** (left) and **4** (right) with atom labeling are shown below the table).

	contact	Distance (Å)	WBI
Receptor **[3]**	**C1-C2/ C4-C5**	1.222	2.886
	C2-C3/ C5-C6	1.466	1.466
	C3-O1	1.475	0.855
	C6-O2	1.474	0.856
Receptor **[4]**	**C1-C2**	1.469	1.084
	C2-C3	1.228	2.614
	C3-C4	1.374	1.239
	C4-C5	1.227	2.608
	C5-C6	1.462	1.088
	C1-O1	1.473	0.859
	C6-O2	1.475	0.853



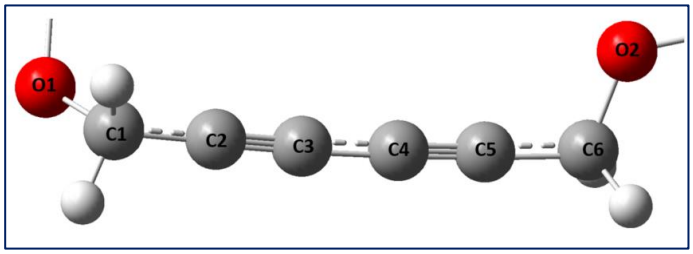
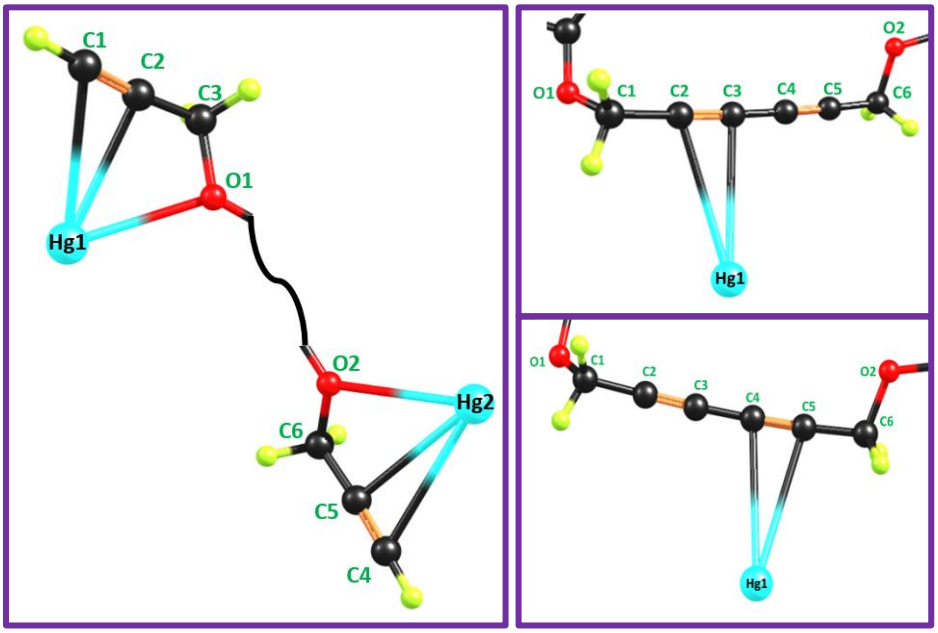


Table S2. The selected distances (Å) and Wiberg Bond Index (WBI) of **[3·2Hg^{2+}]** and **[4·Hg^{2+}]** (involving only terminal alkynes and nearby –*O*–CH_2– as a binding unit) calculated at B3LYP/lanl2dz/cpcm (acetonitrile) level (The zoomed portions of the primary binding core of **[3·2Hg^{2+}]** (left) and **[4·Hg^{2+}]** (right) with atom labelling are shown below the table).

Receptor **[3·2Hg^{2+}]**			*Receptor* **[4·Hg^{2+}]**				
contact	distance(Å)	WBI	contact	Left side alkyne unit		Right side alkyne unit	
				distance(Å)	WBI	distance(Å)	WBI
C1-C2	1.226	2.859					
C2-C3	1.462	1.088	**C1-O1**	1.471	0.861	1.471	0.861
C3-O1	1.502	0.831	**C1-C2**	1.470	1.081	1.470	1.083
C4-C5	1.224	2.866	**C2-C3**	1.229	2.604	1.228	2.604
C5-C6	1.461	1.086	**C3-C4**	1.375	1.237	1.374	1.237
C6-O2	1.496	0.836	**C4-C5**	1.227	2.612	1.228	2.609
C1-Hg1	3.300	0.0157	**C5-C6**	1.463	1.087	1.463	1.085
C2-Hg1	3.019	0.0170	**C6-O2**	1.474	0.855	1.474	0.855
O1-Hg1	2.844	0.0412	**C2-Hg1**	3.697	0.0063	------	------
C4-Hg2	3.402	0.0120	**C3-Hg1**	3.668	0.0072	------	------
C5-Hg2	3.143	0.0128	**C4-Hg1**	------	------	3.654	0.0070
O2-Hg2	2.944	0.0340	**C5-Hg1**	------	------	3.662	0.0063



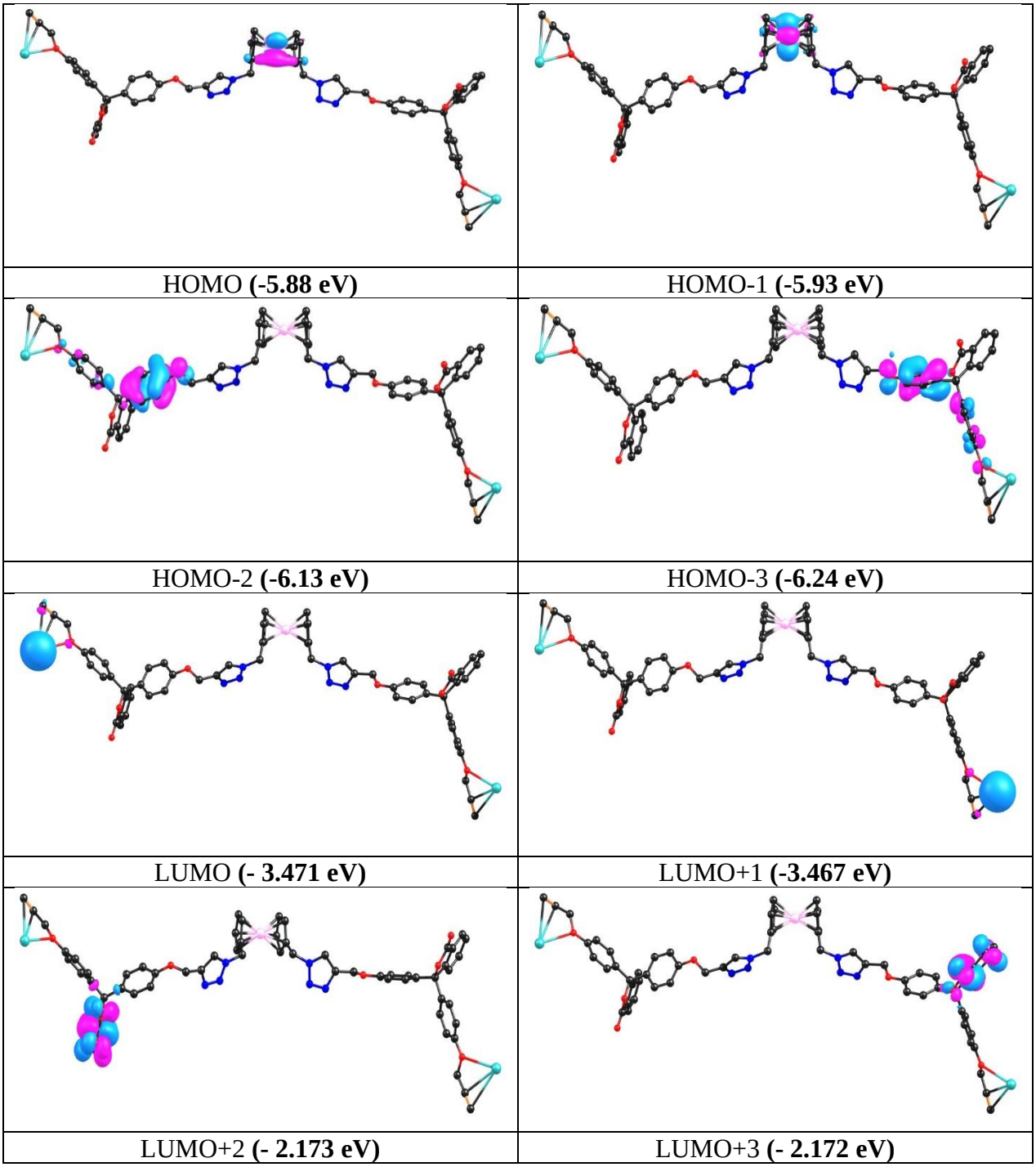


Fig. S28: Frontiers MOs of the free ligand [**3**·2Hg^{2+}] with energy at B3LYP/ lanl2dz / CPCM (acetonitrile) level. (iso value=0.04)

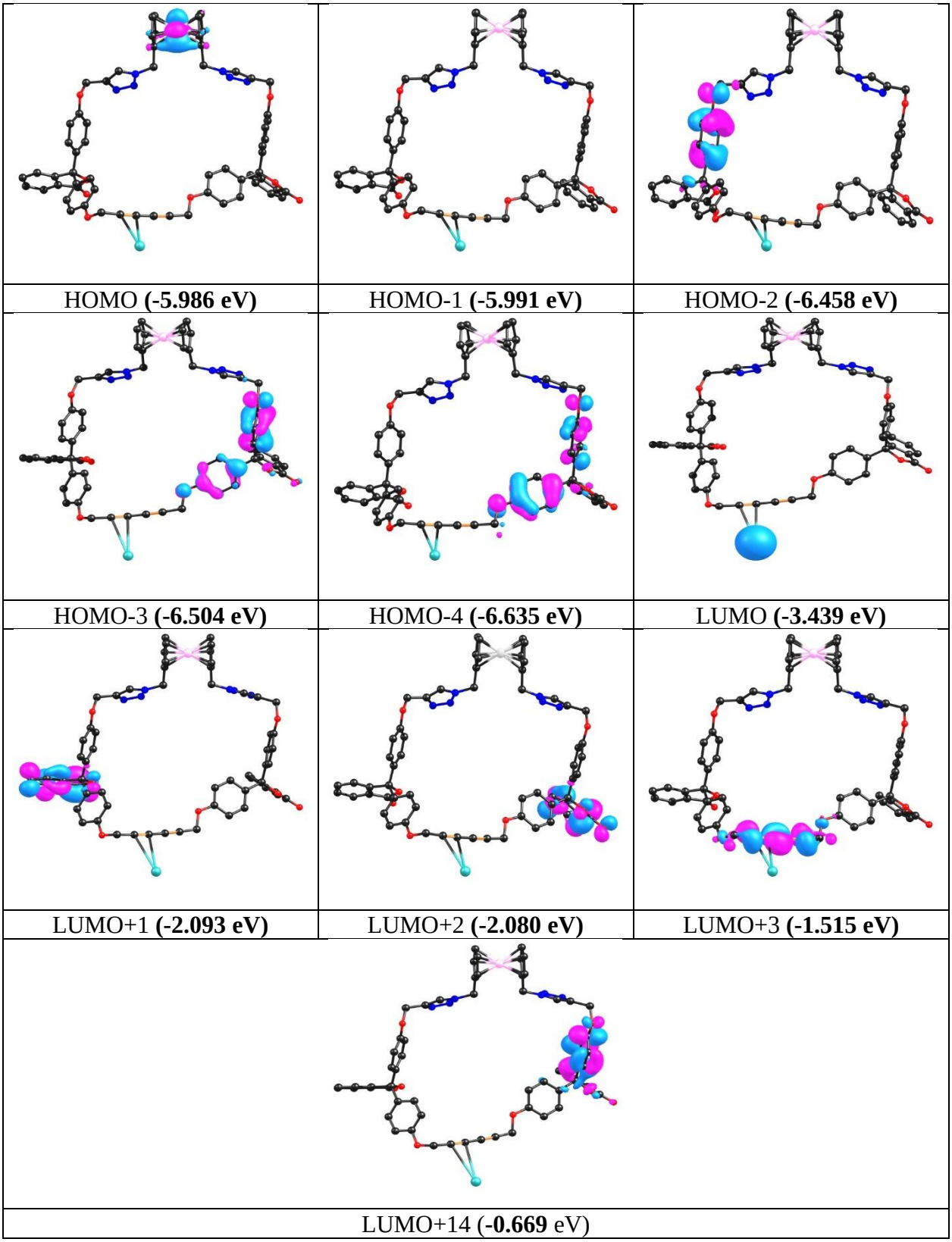


Fig. S29: Frontiers MOs of the free ligand [**4**·Hg^{2+}] with energy at B3LYP/ lanl2dz / CPCM (acetonitrile) level. (iso value=0.04) (left side)

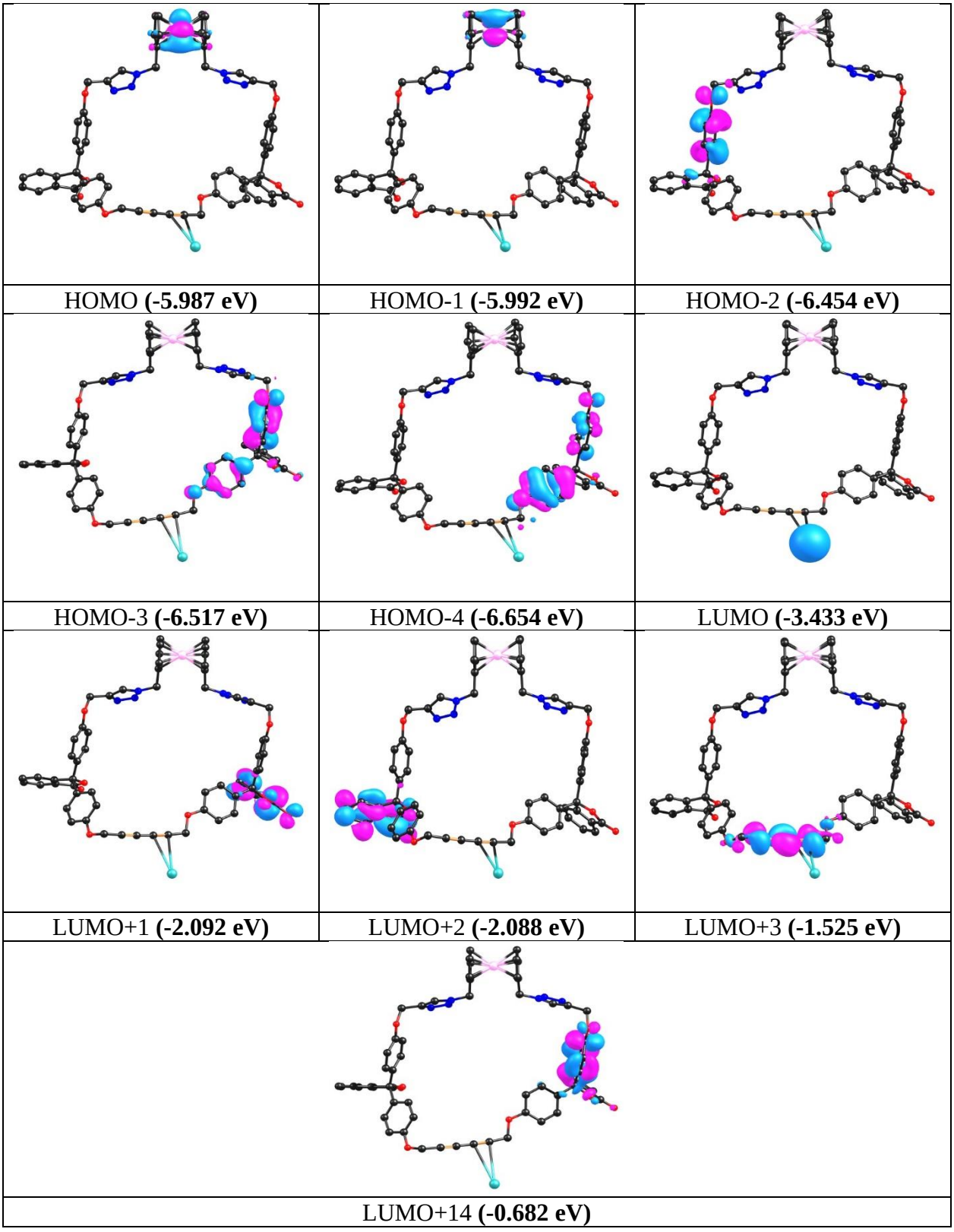


Fig. S30: Frontiers MOs of the free ligand [**4**·Hg^{2+}] with energy at B3LYP/ lanl2dz / CPCM (acetonitrile) level. (iso value=0.04) (right side)

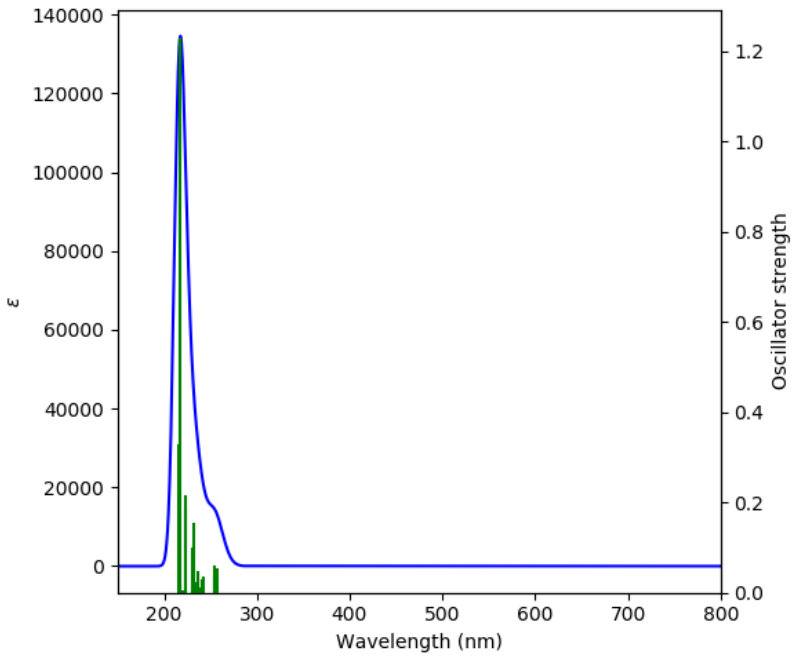


Fig. S31: Calculated absorption spectrum of the ligand/receptor **3**

Table S3. Major excited state transitions of the ligand/receptor **3** with Osc. Strength and λ_{ex}.

λ_{ex} (nm) (Exp.)[a]	**λ_{ex} (nm) (Calc.)**[b]	**Oscillator Strength (*f*)**	**Major Transitions**[c]
227	216.5	1.2303	H-4 → L+10 (32%), H-3 → L+10 (19%)
273	253.6	0.0615	H-27 → L+1 (13%), H-13 → L+1 (29%), H-4 → L+1 (32%)
281	257.1	0.0556	H-28 → L (16%), H-12 → L (15%), H-2 → L (52%)

[a]Experimental wavelength in acetonitrile. [b]TD-DFT calculated wavelength of ligand **3** in acetonitrile. [c]Transitions with greater than 10% contribution are represented.

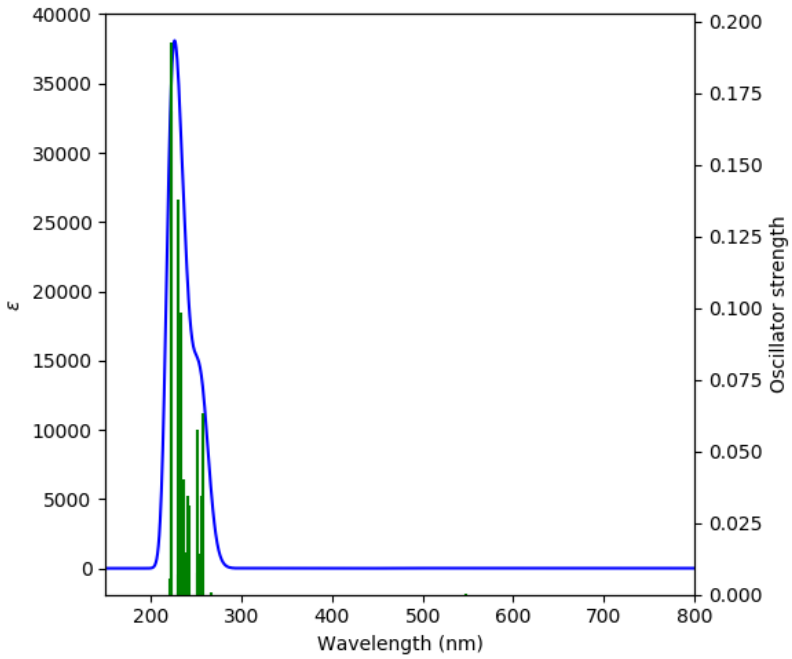


Fig. S32: Calculated absorption spectrum of the ligand/receptor **4**

Table S4. Major excited state transitions of the ligand/receptor **4** with Osc. Strength and λ_{ex}.

λ_{ex} (nm) (Exp.)[a]	**λ_{ex} (nm) (Calc.)**[b]	**Oscillator Strength (*f*)**	**Major Transitions**[c]
227	223.0	0.193	H-18 → L+1 (62%)
273	252.1	0.0575	H-26 → L+1 (24%), H-14 → L+1 (26%), H-4 → L+1 (24%)
281	257.3	0.0633	H-15 → L (16%), H-1 → L (52%)
[a]Experimental wavelength in acetonitrile. [b]TD-DFT calculated wavelength of ligand **4** in acetonitrile. [c]Transitions with greater than 10% contribution are represented.			

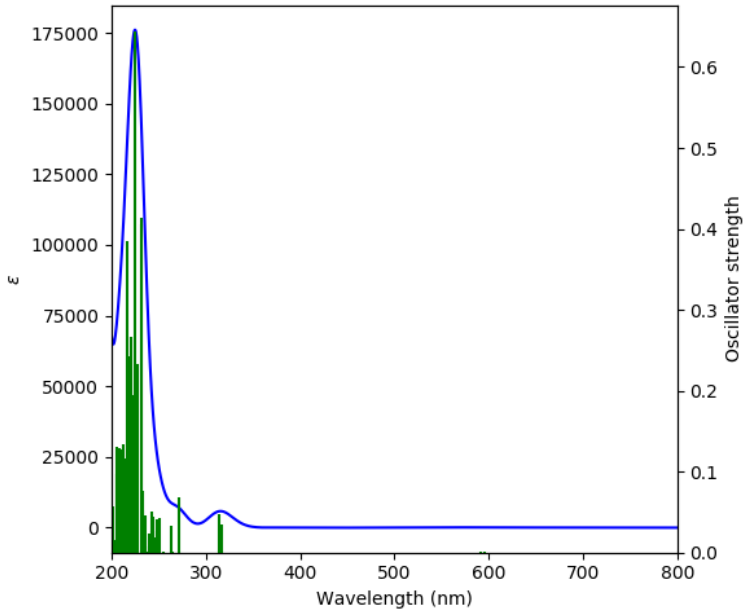


Fig. S33: Calculated absorption spectrum of the complex [**3·2Hg**$^{2+}$]

Table S5. Major excited state transitions of [**3·2Hg**$^{2+}$] (involving only terminal alkynes and nearby –***O***–CH_2– atom as a binding unit) with Osc. Strength and λ_{ex}.

λ_{ex} (nm) (Exp.)[a]	**λ_{ex} (nm) (Calc.)**[b]	**Oscillator Strength (*f*)**	**Major Contributions**[c]
231	225.2	0.6445	H-1 → L+12 (25%), H-4 → L+3 (14%), H-1 → L+9 (18%), H-1 → L+16 (13%)
	231.26	0.4055	H-5 → L+2 (23%), HOMO → L+8 (15%)
274	251.2	0.0426	HOMO → L+5 (18%), HOMO → L+14 (12%), HOMO → L+17 (44%)
	263.6	0.0339	H-1 → L+3 (84%)
281	271.2	0.0676	HOMO → L+2 (88%)
	314.5	0.0468	H-5 → LUMO (62%), HOMO → LUMO (34%)
	316.9	0.0343	H-4 → L+1 (54%), H-1 → L+1 (41%)

[a]Experimental wavelength in acetonitrile. [b]TD-DFT calculated wavelength of complex [**3·2Hg**$^{2+}$] in acetonitrile. [c]Transitions with greater than 10% contribution are presented.

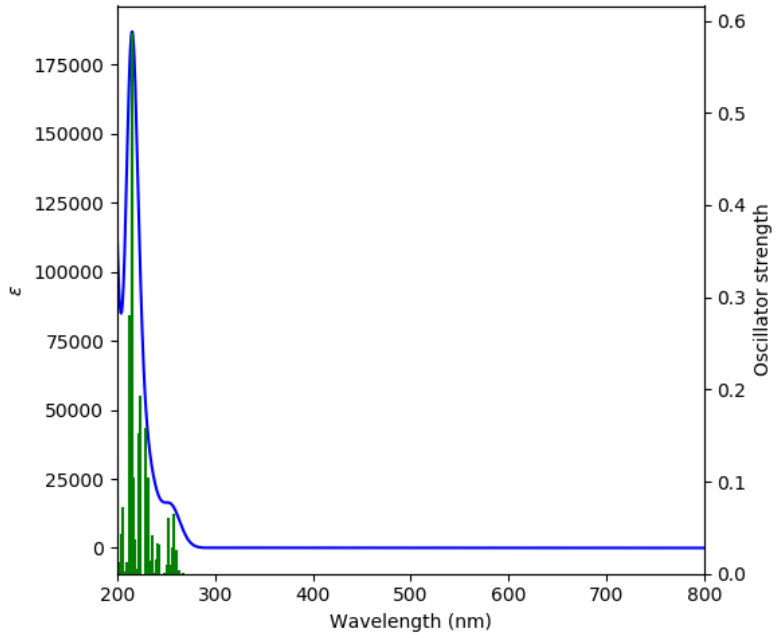


Fig. S34: Calculated absorption spectrum of the complex [**4·Hg**$^{2+}$].

Table S6. Major excited state transitions of [**4·Hg**$^{2+}$] (involving only conjugated alkynes as a binding unit) with Osc. Strength and λ_{ex}.

λ_{ex} (nm) (Exp.)[a]	**λ_{ex} (nm) (Calc.)**[b]	**Oscillator Strength (*f*)**	**Major Contributions**[c]
230	215.5	0.6378	H-4 → L+14 (16%), H-3 → L+14 (41%)
273	251.9	0.0644	H-26 → L+1 (19%), H-14 → L+1 (27%), H-4 → L+1 (27%)
281	257.4	0.0644	H-13 → L+2 (15%), H-2 → L+2 (57%)
[a]Experimental wavelength in acetonitrile. [b]TD-DFT calculated wavelength of complex [**4·Hg**$^{2+}$] (right side alkyne unit) in acetonitrile. [c]Transitions with greater than 10% contribution are presented.			

λ_{ex} (nm) (Exp.)[a]	**λ_{ex} (nm) (Calc.)**[b]	**Oscillator Strength (*f*)**	**Major Contributions**[c]
230	215.4	0.5868	H-4->L+14 (20%), H-3->L+14 (42%)
273	251.9	0.0601	H-25->L+2 (19%), H-14->L+2 (24%), H-4->L+2 (25%)
281	257.4	0.0649	H-13->L+1 (14%), H-2->L+1 (57%)
[a]Experimental wavelength in acetonitrile. [b]TD-DFT calculated wavelength of complex [**4·Hg**$^{2+}$] (left side alkyne unit) in acetonitrile. [c]Transitions with greater than 10% contribution are presented.			

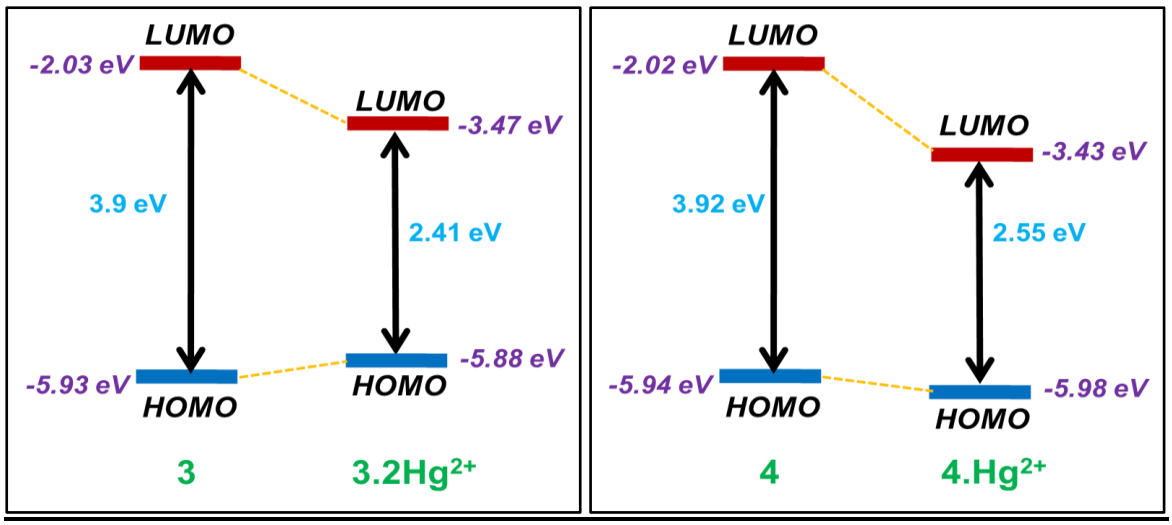


Fig. S35: Energy diagram of the frontier molecular orbitals of receptor **3** and [**3**·2Hg^{2+}] (left) and that of receptor **4** and [**4**·Hg^{2+}] (right) as obtained from DFT calculations.

Table S7. DFT Optimized coordinates of all the compounds.

*Ligand/Receptor **3***

Electronic Energy: -3520.714616 a.u.; **EE + Free Energy Correction**: -3519.857175 a.u.

C	11.835709000	5.892083000	6.052102000	C	4.422036000	-11.468685000	-1.940687000
C	-2.657700000	-20.156587000	-8.863806000	N	5.620088000	-11.694769000	-1.273066000
O	11.094324000	6.666755000	5.040231000	N	6.502542000	-10.745509000	-1.617435000
O	-2.549032000	-18.787468000	-8.325776000	N	5.852974000	-9.904769000	-2.517817000
C	11.116783000	6.201769000	3.717562000	C	4.572182000	-10.327852000	-2.731656000
C	-2.010821000	-18.630942000	-7.042568000	C	14.492475000	6.370673000	-1.778812000
C	10.395375000	6.980805000	2.789663000	C	14.007632000	7.268891000	-2.759628000
C	10.355308000	6.604410000	1.440460000	C	12.624459000	7.414655000	-2.967537000
C	11.022012000	5.441709000	0.993947000	C	11.759772000	6.641407000	-2.175436000
C	11.736941000	4.672915000	1.932934000	C	12.235835000	5.745370000	-1.204339000
C	11.792499000	5.041426000	3.289684000	C	13.612158000	5.600873000	-0.990075000
C	-1.929115000	-17.298759000	-6.580491000	C	10.283816000	6.619606000	-2.176174000
C	-1.401777000	-17.034366000	-5.313322000	O	9.866636000	5.731823000	-1.175746000
C	-0.948828000	-18.084187000	-4.476930000	C	11.060853000	5.065090000	-0.494313000
C	-1.045542000	-19.405387000	-4.950160000	O	9.466107000	7.234032000	-2.880778000
C	-1.566841000	-19.689508000	-6.227260000	C	10.918291000	3.566652000	-0.765538000
C	1.608435000	-20.701715000	-1.596914000	C	9.920987000	2.832516000	-0.077065000
C	0.761288000	-21.012737000	-0.506420000	C	9.703590000	1.479180000	-0.350716000
C	-0.419131000	-20.278914000	-0.292577000	C	10.487824000	0.822787000	-1.326221000
C	-0.717382000	-19.244017000	-1.194254000	C	11.482390000	1.536374000	-2.023822000
C	0.117113000	-18.934510000	-2.280824000	C	11.683738000	2.900759000	-1.740398000
C	1.296500000	-19.658978000	-2.494128000	O	10.197907000	-0.529894000	-1.521957000
C	-1.867519000	-18.319184000	-1.185014000	C	10.981160000	-1.273371000	-2.536241000
O	-1.708491000	-17.425218000	-2.252277000	C	10.526004000	-2.691578000	-2.521947000
C	-0.459438000	-17.751469000	-3.065829000	N	11.120085000	-3.647329000	-1.705889000
O	-2.844658000	-18.250487000	-0.421516000	N	10.512022000	-4.827528000	-1.895017000
C	0.477408000	-16.536563000	-3.002000000	N	9.515761000	-4.615296000	-2.844856000
C	1.536473000	-16.424038000	-3.933668000	C	9.506187000	-3.310507000	-3.247456000
C	2.460480000	-15.376007000	-3.847776000	C	8.671484000	-5.751659000	-3.289190000
C	2.339826000	-14.411537000	-2.823911000	H	12.899193000	5.850246000	5.780276000
C	1.285333000	-14.504092000	-1.893575000	H	11.442364000	4.867413000	6.095654000
C	0.368382000	-15.568852000	-1.987564000	H	-3.297714000	-20.761871000	-8.207746000
O	3.313502000	-13.406711000	-2.823566000	H	-1.661265000	-20.616510000	-8.907383000
C	3.244933000	-12.366133000	-1.772010000	H	9.876128000	7.869076000	3.136860000

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H	12.353239000	4.420622000	3.979875000	H	5.214822000	-7.817918000	-5.585583000
H	-2.279404000	-16.495371000	-7.221281000	C	6.096128000	-8.439283000	-5.671222000
H	-1.344028000	-16.005826000	-4.968758000	H	10.723981000	-7.406747000	-4.682868000
H	-0.714293000	-20.235308000	-4.334433000	C	8.891015000	-6.094225000	-4.737186000
H	-1.617759000	-20.721590000	-6.556212000	C	9.961613000	-6.909182000	-5.266779000
H	2.518148000	-21.277273000	-1.744862000	Fe	8.088423000	-7.735260000	-5.806762000
H	1.029731000	-21.820959000	0.167607000	C	7.846702000	-9.705900000	-6.554729000
H	-1.079483000	-20.498290000	0.541217000	C	6.694404000	-8.905324000	-6.896378000
H	1.961145000	-19.433244000	-3.322167000	C	8.103877000	-5.618781000	-5.853655000
H	1.638764000	-17.149643000	-4.735950000	C	9.836577000	-6.932964000	-6.701907000
H	3.274262000	-15.289476000	-4.561524000	H	8.516801000	-10.185631000	-7.254336000
H	1.161915000	-13.771552000	-1.103481000	H	6.349599000	-8.681990000	-7.896266000
H	-0.441906000	-15.627522000	-1.269056000	C	8.687908000	-6.136440000	-7.064790000
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H	3.884697000	-9.823835000	-3.390158000	H	7.231159000	-4.983361000	-5.784635000
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H	12.232554000	8.102298000	-3.711122000	C	6.584532000	-8.755557000	-3.104677000
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H	9.309932000	3.324158000	0.674581000	H	7.502976000	-8.674180000	-2.517193000
H	8.938021000	0.917108000	0.175577000	C	-3.238680000	-20.076392000	-10.206990000
H	12.097396000	1.059114000	-2.778627000	C	11.669660000	6.554100000	7.349317000
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H	10.817864000	-0.816649000	-3.519389000	C	11.552501000	7.080473000	8.446094000
H	12.045789000	-1.216863000	-2.279469000	H	-4.141596000	-20.017166000	-12.311232000
H	8.819484000	-2.922909000	-3.981293000	H	11.448580000	7.541854000	9.404106000
C	6.878066000	-8.950868000	-4.567346000				

*Ligand/Receptor **4***

Electronic Energy: -3519.532780 a.u.; **EE + Free Energy Correction**: -3518.682147 a.u.

C	8.865360000	-6.934177000	8.709249000	O	4.182768000	-12.777621000	8.999989000
C	3.775666000	-11.371205000	8.842008000	C	10.353864000	-6.115059000	6.912241000
O	9.363515000	-7.018496000	7.323387000	C	4.859725000	-13.423032000	7.954436000

C	10.951225000	-5.143748000	7.738947000	C	15.327957000	-5.336192000	5.032281000
C	11.931524000	-4.287452000	7.199869000	C	14.796604000	-2.072753000	6.640653000
C	12.314008000	-4.378903000	5.849166000	O	13.515426000	-2.228904000	6.095034000
C	11.705783000	-5.363950000	5.036739000	C	13.423715000	-3.497092000	5.256867000
C	10.736644000	-6.227361000	5.559941000	O	15.097793000	-1.073365000	7.313373000
C	5.251288000	-12.806141000	6.749492000	C	13.118304000	-3.043059000	3.826514000
C	5.930061000	-13.561970000	5.778145000	C	11.915956000	-2.331269000	3.592400000
C	6.219800000	-14.927128000	5.977765000	C	11.577592000	-1.892416000	2.309521000
C	5.817659000	-15.525522000	7.194569000	C	12.435626000	-2.170397000	1.221269000
C	5.144033000	-14.785816000	8.174686000	C	13.637104000	-2.870900000	1.434877000
C	6.130435000	-19.476695000	5.065854000	C	13.971511000	-3.292578000	2.737761000
C	7.395523000	-19.979322000	5.454637000	O	12.000303000	-1.687073000	-0.018070000
C	8.473435000	-19.101773000	5.668212000	C	12.700970000	-2.088442000	-1.257700000
C	8.243937000	-17.728426000	5.483082000	C	12.457920000	-3.521094000	-1.624407000
C	6.990963000	-17.225086000	5.097619000	N	13.473330000	-4.470065000	-1.621488000
C	5.915063000	-18.094926000	4.881843000	N	12.968372000	-5.659840000	-1.983758000
C	9.193217000	-16.607921000	5.632185000	N	11.610237000	-5.460916000	-2.214449000
O	8.516079000	-15.424547000	5.308002000	C	11.272512000	-4.154144000	-2.006747000
C	7.055792000	-15.699970000	4.954410000	C	10.763682000	-6.601258000	-2.644483000
O	10.387293000	-16.598961000	5.973476000	H	8.502573000	-5.917517000	8.916227000
C	6.838678000	-15.280869000	3.493237000	H	9.676224000	-7.169131000	9.412625000
C	5.525019000	-15.120558000	2.993043000	H	3.089756000	-11.199613000	9.676318000
C	5.301836000	-14.825921000	1.642183000	H	3.217547000	-11.246810000	7.904499000
C	6.394877000	-14.686423000	0.759908000	H	10.675495000	-5.037360000	8.782789000
C	7.710080000	-14.835954000	1.241967000	H	12.379848000	-3.535807000	7.840882000
C	7.917663000	-15.136994000	2.601774000	H	11.977642000	-5.452000000	3.988932000
O	6.059158000	-14.397928000	-0.569417000	H	10.264362000	-6.981407000	4.937763000
C	7.093393000	-14.462630000	-1.625930000	H	5.051587000	-11.758001000	6.557379000
C	7.931449000	-13.225005000	-1.736747000	H	6.236674000	-13.071149000	4.859513000
N	9.241335000	-13.172392000	-1.272969000	H	6.027265000	-16.573063000	7.387362000
N	9.757252000	-11.963114000	-1.537223000	H	4.834089000	-15.246015000	9.107857000
N	8.758021000	-11.236233000	-2.178076000	H	5.309386000	-20.170119000	4.905381000
C	7.627712000	-11.990135000	-2.315777000	H	7.529783000	-21.048950000	5.586678000
C	16.649678000	-5.669964000	5.395381000	H	9.451811000	-19.467539000	5.965541000
C	17.437571000	-4.800582000	6.186683000	H	4.938334000	-17.727433000	4.582692000
C	16.909790000	-3.577692000	6.638022000	H	4.669685000	-15.220464000	3.655619000
C	15.592782000	-3.258480000	6.269211000	H	4.293378000	-14.706767000	1.257416000
C	14.810254000	-4.111496000	5.472694000	H	8.566157000	-14.702411000	0.590162000

H	8.934595000	-15.241660000	2.963577000	C	11.108837000	-6.865046000	-5.235710000
H	7.732570000	-15.337863000	-1.464102000	Fe	9.274321000	-7.921666000	-5.221978000
H	6.508407000	-14.611429000	-2.536080000	C	8.990747000	-9.668190000	-6.391960000
H	6.732833000	-11.630007000	-2.794976000	C	7.712439000	-9.075465000	-6.075547000
H	17.070555000	-6.614939000	5.062850000	C	9.082924000	-5.921490000	-4.553071000
H	18.451774000	-5.086212000	6.450125000	C	10.349813000	-6.536146000	-6.415178000
H	17.493687000	-2.902372000	7.256386000	H	9.393785000	-9.816328000	-7.384025000
H	14.737031000	-6.022362000	4.433645000	H	6.990102000	-8.703878000	-6.788715000
H	11.243283000	-2.123765000	4.419921000	C	9.097339000	-5.953930000	-5.993476000
H	10.656956000	-1.345685000	2.128527000	H	10.656449000	-6.712264000	-7.436720000
H	14.306231000	-3.106815000	0.615465000	H	8.302882000	-5.616019000	-6.643995000
H	14.905404000	-3.826142000	2.879755000	H	8.284543000	-5.541817000	-3.929729000
H	12.281583000	-1.410536000	-2.004030000	H	11.379437000	-7.490269000	-2.482515000
H	13.776048000	-1.897113000	-1.169388000	H	9.899949000	-6.647413000	-1.973704000
H	10.271876000	-3.775518000	-2.131434000	C	9.030677000	-9.839141000	-2.601102000
C	8.772115000	-9.624214000	-4.066512000	H	8.408997000	-9.171451000	-1.994990000
H	10.618661000	-10.467294000	-5.050590000	H	10.078743000	-9.668002000	-2.341821000
C	9.646819000	-10.004086000	-5.153971000	C	4.897373000	-10.424227000	8.898290000
H	6.730542000	-8.668147000	-4.085226000	C	7.772513000	-7.897504000	8.834152000
C	7.576717000	-9.048430000	-4.641549000	C	5.817421000	-9.610898000	8.918896000
H	12.092840000	-7.313238000	-5.212479000	C	6.851247000	-8.706540000	8.891602000
C	10.328593000	-6.484305000	-4.079727000				

*Complex [**3**·2Hg^{2+}]*

Electronic Energy: -3604.849652 a.u.; **EE + Free Energy Correction**: -3604.012116 a.u.

C	13.101785000	5.476790000	5.866466000	C	-2.683362000	-18.209224000	-4.295049000
C	-3.114054000	-21.120483000	-8.229379000	C	-1.329818000	-18.600569000	-4.069835000
O	12.339080000	6.378993000	4.949447000	C	-0.747717000	-19.578180000	-4.916414000
O	-3.697107000	-20.395441000	-7.050797000	C	-1.497866000	-20.196960000	-5.922513000
C	12.191563000	6.022716000	3.612105000	C	2.530081000	-20.081090000	-1.810314000
C	-2.849066000	-19.809834000	-6.113371000	C	2.073848000	-20.433825000	-0.519679000
C	11.163667000	6.704245000	2.912692000	C	0.822256000	-19.976256000	-0.055010000
C	10.958396000	6.448363000	1.557746000	C	0.060094000	-19.176327000	-0.914963000
C	11.782713000	5.519844000	0.867051000	C	0.494340000	-18.840089000	-2.213002000
C	12.784449000	4.817436000	1.592069000	C	1.749800000	-19.279421000	-2.668829000
C	13.003234000	5.068365000	2.949668000	C	-1.249764000	-18.551440000	-0.636816000
C	-3.435098000	-18.804763000	-5.303566000	O	-1.592216000	-17.793293000	-1.814967000

C	-0.584972000	-17.969848000	-2.881750000	C	7.482024000	-4.795333000	-4.001673000
O	-1.985617000	-18.571570000	0.336926000	H	14.156858000	5.459312000	5.567781000
C	-0.067871000	-16.582368000	-3.272238000	H	12.676515000	4.468418000	5.785475000
C	0.888679000	-16.419283000	-4.324916000	H	-2.563331000	-22.002569000	-7.883299000
C	1.411854000	-15.169759000	-4.617597000	H	-2.434311000	-20.432101000	-8.746216000
C	0.988576000	-14.021121000	-3.866872000	H	10.548431000	7.423341000	3.444851000
C	-0.001670000	-14.165756000	-2.840737000	H	10.176531000	6.966629000	1.015790000
C	-0.522642000	-15.424291000	-2.566815000	H	13.398628000	4.071063000	1.098247000
O	1.574169000	-12.855966000	-4.220036000	H	13.788451000	4.530287000	3.470145000
C	1.380185000	-11.572184000	-3.441061000	H	-4.470255000	-18.523590000	-5.470368000
C	2.611474000	-10.753583000	-3.559481000	H	-3.141518000	-17.477029000	-3.639757000
N	3.727946000	-11.048759000	-2.778227000	H	0.275392000	-19.902158000	-4.760217000
N	4.666832000	-10.135562000	-2.991896000	H	-1.035868000	-20.968865000	-6.529318000
N	4.141794000	-9.227127000	-3.927555000	H	3.502623000	-20.431161000	-2.144172000
C	2.877421000	-9.594665000	-4.294009000	H	2.697178000	-21.050805000	0.120537000
C	14.986163000	6.203761000	-2.375371000	H	0.457721000	-20.224471000	0.937579000
C	14.477707000	7.165756000	-3.276749000	H	2.143179000	-19.009472000	-3.644384000
C	13.104312000	7.479955000	-3.281185000	H	1.217601000	-17.274633000	-4.905893000
C	12.276374000	6.803488000	-2.375314000	H	2.154806000	-15.026313000	-5.395251000
C	12.769208000	5.828725000	-1.487021000	H	-0.358525000	-13.309006000	-2.279992000
C	14.140150000	5.526975000	-1.471599000	H	-1.274543000	-15.546543000	-1.796131000
C	10.827050000	6.998198000	-2.162432000	H	0.501067000	-11.082541000	-3.870625000
O	10.454493000	6.122567000	-1.086077000	H	1.207917000	-11.834716000	-2.393447000
C	11.600624000	5.294839000	-0.641731000	H	2.276646000	-9.041139000	-4.997564000
O	10.005865000	7.726535000	-2.701430000	H	16.050330000	5.984894000	-2.375834000
C	11.191805000	3.836910000	-0.898239000	H	15.153061000	7.672019000	-3.959928000
C	9.828607000	3.471464000	-0.675287000	H	12.692228000	8.227586000	-3.952660000
C	9.383703000	2.187478000	-0.956265000	H	14.569888000	4.808979000	-0.779059000
C	10.294082000	1.215061000	-1.470977000	H	9.128409000	4.223828000	-0.330171000
C	11.666439000	1.554973000	-1.664257000	H	8.347081000	1.898866000	-0.816854000
C	12.097972000	2.850377000	-1.373818000	H	12.374486000	0.828815000	-2.048452000
O	9.745948000	-0.000455000	-1.756834000	H	13.134628000	3.107244000	-1.561903000
C	10.576068000	-1.099701000	-2.349204000	H	10.995301000	-0.728897000	-3.291887000
C	9.712881000	-2.292077000	-2.551816000	H	11.377198000	-1.340648000	-1.641744000
N	9.658197000	-3.299207000	-1.591198000	H	8.663344000	-2.153147000	-4.547574000
N	8.844709000	-4.263632000	-2.007520000	C	5.953647000	-8.449239000	-5.428057000
N	8.360428000	-3.864766000	-3.265623000	H	7.413240000	-9.772103000	-4.340142000
C	8.890033000	-2.654014000	-3.620353000	C	7.097187000	-9.315106000	-5.267856000

H	5.117764000	-7.441160000	-7.266385000	H	7.477380000	-4.687786000	-6.996885000
C	5.869957000	-8.078592000	-6.820685000	H	7.076175000	-5.462615000	-3.235244000
H	9.587229000	-6.887470000	-3.839750000	H	6.655952000	-4.227150000	-4.442472000
C	8.242771000	-5.556709000	-5.061862000	C	4.982348000	-8.077216000	-4.334773000
C	9.269510000	-6.541137000	-4.813980000	H	4.316627000	-7.268299000	-4.651861000
Fe	7.766119000	-7.431722000	-6.060086000	H	5.505614000	-7.760528000	-3.427282000
C	7.702233000	-9.497718000	-6.560856000	C	-4.217348000	-21.503713000	-9.108449000
C	6.946057000	-8.732011000	-7.522100000	C	12.952232000	5.983237000	7.229082000
C	8.150683000	-5.365692000	-6.488898000	C	-5.060147000	-21.840381000	-9.932839000
C	9.829708000	-6.931492000	-6.081633000	C	12.857502000	6.317100000	8.403255000
H	8.574216000	-10.100085000	-6.773309000	H	-5.782200000	-22.130749000	-10.670449000
H	7.148922000	-8.661935000	-8.581454000	H	12.773042000	6.589547000	9.435591000
C	9.135711000	-6.208135000	-7.119361000	Hg	-6.182870000	-21.759693000	-6.830921000
H	10.628909000	-7.644060000	-6.229550000	Hg	12.749737000	8.972730000	6.279221000
H	9.324088000	-6.280385000	-8.181255000				

*Complex [**4·Hg**$^{2+}$**] (left side)*

Electronic Energy: -3562.039179 a.u.; **EE + Free Energy Correction**: -3561.192992 a.u.

C	8.788299000	-6.947029000	8.661317000	C	8.590952000	-19.031723000	5.715043000
C	3.684837000	-11.370941000	8.729519000	C	8.332450000	-17.666329000	5.510291000
O	9.287013000	-7.030078000	7.276768000	C	7.074810000	-17.197312000	5.097633000
O	4.105042000	-12.770057000	8.904534000	C	6.023752000	-18.094744000	4.872923000
C	10.280545000	-6.127228000	6.868913000	C	9.252685000	-16.522221000	5.661362000
C	4.815302000	-13.412200000	7.877448000	O	8.553789000	-15.358960000	5.309973000
C	10.877656000	-5.159001000	7.699088000	C	7.106391000	-15.672974000	4.937794000
C	11.859337000	-4.302198000	7.163463000	O	10.439925000	-16.480412000	6.023085000
C	12.243646000	-4.390654000	5.813078000	C	6.900306000	-15.274704000	3.469348000
C	11.636271000	-5.373667000	4.997631000	C	5.590487000	-15.141747000	2.951543000
C	10.665296000	-6.237382000	5.517248000	C	5.379151000	-14.867046000	1.594558000
C	5.227291000	-12.795179000	6.679596000	C	6.480505000	-14.720842000	0.723750000
C	5.936801000	-13.547086000	5.727396000	C	7.792012000	-14.844170000	1.223310000
C	6.238235000	-14.907712000	5.940157000	C	7.987732000	-15.125202000	2.589071000
C	5.815831000	-15.505723000	7.150016000	O	6.156422000	-14.453054000	-0.612573000
C	5.110503000	-14.770012000	8.110956000	C	7.203906000	-14.514026000	-1.656473000
C	6.268421000	-19.468930000	5.076333000	C	8.026417000	-13.266290000	-1.769864000
C	7.537937000	-19.936924000	5.492870000	N	9.329497000	-13.191338000	-1.290247000

N	9.832358000	-11.977834000	-1.560020000	H	4.784264000	-15.230230000	9.038529000
N	8.831671000	-11.270926000	-2.220596000	H	5.467124000	-20.183528000	4.909094000
C	7.713429000	-12.041362000	-2.364937000	H	7.695226000	-21.001537000	5.639149000
C	16.583061000	-5.675444000	5.373386000	H	9.572380000	-19.371017000	6.032944000
C	17.366483000	-4.806086000	6.169123000	H	5.044301000	-17.753835000	4.551996000
C	16.835076000	-3.584711000	6.620328000	H	4.728940000	-15.248090000	3.605033000
C	15.518989000	-3.266979000	6.246972000	H	4.373735000	-14.768964000	1.196121000
C	14.740921000	-4.120038000	5.446124000	H	8.653730000	-14.705654000	0.580046000
C	15.262211000	-5.343163000	5.005681000	H	9.001801000	-15.209731000	2.964055000
C	14.719713000	-2.082864000	6.616802000	H	7.852787000	-15.378856000	-1.478278000
O	13.440975000	-2.239830000	6.065249000	H	6.631568000	-14.679850000	-2.571681000
C	13.354506000	-3.507149000	5.225201000	H	6.820028000	-11.698061000	-2.859012000
O	15.016269000	-1.084302000	7.292694000	H	17.006865000	-6.619058000	5.040733000
C	13.054512000	-3.052387000	3.794044000	H	18.380190000	-5.090416000	6.435821000
C	11.850422000	-2.345451000	3.554140000	H	17.415676000	-2.909337000	7.241722000
C	11.517577000	-1.905819000	2.270069000	H	14.674902000	-6.029007000	4.403107000
C	12.383272000	-2.177831000	1.186330000	H	11.172096000	-2.142095000	4.378095000
C	13.586919000	-2.872813000	1.405948000	H	10.595624000	-1.362809000	2.084627000
C	13.915468000	-3.295508000	2.709901000	H	14.262016000	-3.103928000	0.590123000
O	11.952751000	-1.695135000	-0.054734000	H	14.851079000	-3.824811000	2.856392000
C	12.664096000	-2.089560000	-1.290814000	H	12.243842000	-1.414116000	-2.038835000
C	12.434651000	-3.523687000	-1.660270000	H	13.737003000	-1.889722000	-1.195438000
N	13.456315000	-4.465877000	-1.645597000	H	10.256002000	-3.793050000	-2.190695000
N	12.963194000	-5.659291000	-2.011743000	C	8.834941000	-9.667699000	-4.117620000
N	11.606257000	-5.469731000	-2.257245000	H	10.699768000	-10.483266000	-5.090386000
C	11.257663000	-4.165001000	-2.054665000	C	9.721089000	-10.036116000	-5.199745000
C	10.772022000	-6.617432000	-2.691701000	H	6.778312000	-8.744517000	-4.149078000
H	8.432396000	-5.928777000	8.872691000	C	7.633359000	-9.112434000	-4.700140000
H	9.595505000	-7.191431000	9.365712000	H	12.124422000	-7.309274000	-5.253014000
H	2.968528000	-11.206970000	9.539057000	C	10.342770000	-6.505806000	-4.129033000
H	3.157365000	-11.254002000	7.773426000	C	11.133935000	-6.875889000	-5.281088000
H	10.601250000	-5.055104000	8.743013000	Fe	9.315723000	-7.960009000	-5.274123000
H	12.307256000	-3.552499000	7.806983000	C	9.066071000	-9.713529000	-6.441810000
H	11.910124000	-5.459869000	3.950236000	C	7.776815000	-9.140729000	-6.133338000
H	10.193558000	-6.989637000	4.892507000	C	9.090999000	-5.962067000	-4.608581000
H	5.019950000	-11.750292000	6.477589000	C	10.375463000	-6.559423000	-6.464266000
H	6.258267000	-13.057110000	4.813391000	H	9.476485000	-9.857440000	-7.431464000
H	6.033564000	-16.549744000	7.352322000	H	7.052258000	-8.782593000	-6.851119000

C	9.112497000	-5.995725000	-6.048868000	H	8.458668000	-9.209489000	-2.049836000
H	10.689379000	-6.731790000	-7.484229000	H	10.135209000	-9.689007000	-2.387847000
H	8.316164000	-5.670200000	-6.703396000	C	4.794541000	-10.410560000	8.819234000
H	8.284150000	-5.593766000	-3.989329000	C	7.687291000	-7.902487000	8.780682000
H	11.395201000	-7.500599000	-2.526258000	C	5.719220000	-9.601508000	8.852305000
H	9.905276000	-6.671478000	-2.025353000	C	6.759623000	-8.704358000	8.832686000
C	9.090119000	-9.873117000	-2.650338000	Hg	3.648622000	-8.146312000	11.507892000

*Complex **[4·Hg^{2+}]** (right side)*

Electronic Energy: -3562.039334 a.u.; **EE + Free Energy Correction**: -3561.194498 a.u.

C	8.709781000	-6.845185000	8.683286000	C	5.395711000	-14.862730000	1.595340000
C	3.680365000	-11.351822000	8.711536000	C	6.494727000	-14.716901000	0.721558000
O	9.211530000	-6.952444000	7.301665000	C	7.807704000	-14.833956000	1.218818000
O	4.112683000	-12.746439000	8.893652000	C	8.007201000	-15.107517000	2.585540000
C	10.221908000	-6.071682000	6.886115000	O	6.166892000	-14.455877000	-0.615224000
C	4.827598000	-13.387688000	7.869798000	C	7.212488000	-14.516364000	-1.660874000
C	10.832936000	-5.103896000	7.706348000	C	8.032995000	-13.267511000	-1.777282000
C	11.833551000	-4.273114000	7.164432000	N	9.339005000	-13.192768000	-1.305704000
C	12.222321000	-4.386993000	5.817389000	N	9.839415000	-11.978375000	-1.575977000
C	11.598749000	-5.367648000	5.011275000	N	8.834183000	-11.270698000	-2.228720000
C	10.609316000	-6.205934000	5.537373000	C	7.715517000	-12.041527000	-2.367797000
C	5.237329000	-12.772468000	6.670153000	C	16.519993000	-5.794775000	5.367180000
C	5.951919000	-13.523589000	5.721156000	C	17.330012000	-4.946493000	6.159083000
C	6.260838000	-14.881813000	5.938769000	C	16.835109000	-3.709360000	6.608868000
C	5.841177000	-15.477917000	7.150545000	C	15.527678000	-3.354786000	6.238148000
C	5.130831000	-14.742952000	8.108302000	C	14.723566000	-4.187045000	5.441261000
C	6.319633000	-19.446381000	5.096016000	C	15.208298000	-5.425530000	5.002062000
C	7.592591000	-19.904227000	5.513361000	C	14.763428000	-2.147441000	6.606982000
C	8.639999000	-18.991255000	5.730165000	O	13.479320000	-2.268892000	6.058477000
C	8.372511000	-17.628515000	5.519312000	C	13.354447000	-3.535680000	5.222795000
C	7.111421000	-17.169587000	5.105857000	O	15.089767000	-1.156268000	7.279965000
C	6.065900000	-18.074770000	4.886477000	C	13.062620000	-3.078346000	3.790914000
C	9.285501000	-16.477753000	5.663805000	C	11.868361000	-2.356002000	3.547885000
O	8.578892000	-15.320793000	5.307507000	C	11.544759000	-1.911593000	2.263128000
C	7.132743000	-15.645901000	4.938951000	C	12.410132000	-2.193891000	1.181772000
O	10.472912000	-16.426668000	6.023996000	C	13.604632000	-2.903630000	1.404586000
C	6.922138000	-15.255939000	3.468923000	C	13.923988000	-3.331197000	2.709194000
C	5.610803000	-15.130217000	2.953184000	O	11.988666000	-1.706061000	-0.060265000

C	12.699879000	-2.106673000	-1.294421000	H	11.190010000	-2.144619000	4.369832000
C	12.459236000	-3.538757000	-1.664750000	H	10.630145000	-1.357140000	2.075272000
N	13.473954000	-4.488386000	-1.650719000	H	14.279203000	-3.142571000	0.590578000
N	12.972112000	-5.677916000	-2.017639000	H	14.852402000	-3.872412000	2.858167000
N	11.616602000	-5.478258000	-2.262899000	H	12.287621000	-1.427428000	-2.043453000
C	11.277513000	-4.171175000	-2.059435000	H	13.774241000	-1.916283000	-1.195975000
C	10.773858000	-6.619969000	-2.696607000	H	10.278512000	-3.791989000	-2.195066000
H	8.351097000	-5.823855000	8.874108000	C	8.824199000	-9.661520000	-4.120986000
H	9.515854000	-7.074380000	9.394192000	H	10.678972000	-10.481238000	-5.109440000
H	2.963186000	-11.188506000	9.520906000	C	9.701255000	-10.030041000	-5.210464000
H	3.151745000	-11.244138000	7.755095000	H	6.770958000	-8.730478000	-4.135060000
H	10.553269000	-4.980733000	8.747329000	C	7.620678000	-9.099933000	-4.693286000
H	12.293650000	-3.523891000	7.799839000	H	12.114875000	-7.313448000	-5.263683000
H	11.874684000	-5.471618000	3.965968000	C	10.340582000	-6.503913000	-4.132366000
H	10.125822000	-6.956928000	4.920178000	C	11.126161000	-6.875790000	-5.287676000
H	5.023861000	-11.729545000	6.464473000	Fe	9.303495000	-7.952291000	-5.275863000
H	6.271134000	-13.034998000	4.805600000	C	9.038650000	-9.701274000	-6.446883000
H	6.064668000	-16.519978000	7.356652000	C	7.753858000	-9.124417000	-6.127541000
H	4.806329000	-15.201740000	9.037189000	C	9.089447000	-5.954299000	-4.606826000
H	5.522780000	-20.166911000	4.933030000	C	10.364897000	-6.554522000	-6.467776000
H	7.756890000	-20.967111000	5.664462000	H	9.441466000	-9.843816000	-7.439851000
H	9.623908000	-19.322781000	6.048593000	H	7.025576000	-8.761411000	-6.839077000
H	5.083941000	-17.741572000	4.565083000	C	9.105752000	-5.986112000	-6.047220000
H	4.751059000	-15.236506000	3.609026000	H	10.674502000	-6.726848000	-7.489063000
H	4.389137000	-14.769859000	1.198588000	H	8.308495000	-5.656389000	-6.698512000
H	8.667654000	-14.696295000	0.573017000	H	8.286342000	-5.583463000	-3.984230000
H	9.022366000	-15.186917000	2.958702000	H	11.392165000	-7.507114000	-2.534272000
H	7.863342000	-15.379772000	-1.482848000	H	9.908808000	-6.669681000	-2.027698000
H	6.638672000	-14.684412000	-2.574751000	C	9.089218000	-9.871606000	-2.656110000
H	6.818797000	-11.697567000	-2.855372000	H	8.461660000	-9.209878000	-2.049459000
H	16.915770000	-6.750821000	5.035495000	H	10.135980000	-9.688115000	-2.399935000
H	18.335833000	-5.259195000	6.423866000	C	4.779884000	-10.380708000	8.799074000
H	17.436621000	-3.049653000	7.227177000				
H	14.599876000	-6.095319000	4.402307000				

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