# Anthracene-based ferrocenylselenoethers: syntheses, crystal structures, Cu(I) complexes and sensoring property

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**Fig. S1:** $^{1}$H NMR spectrum of **L3,** $CDCl_3$, 298 K.

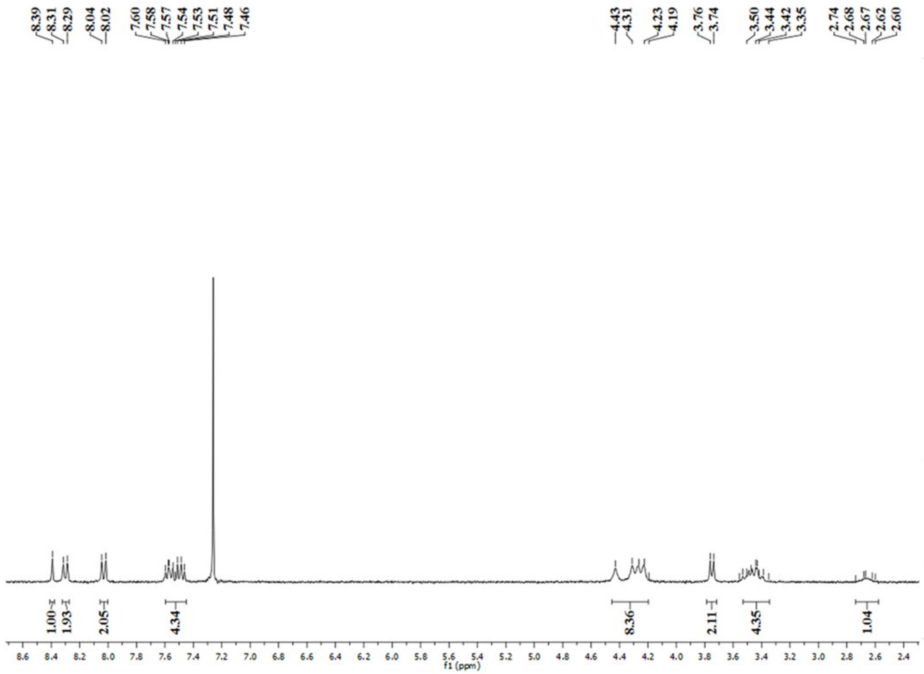


**Fig. S2:** $^{1}$H NMR spectrum of **L4,** $CDCl_3$, 298 K.

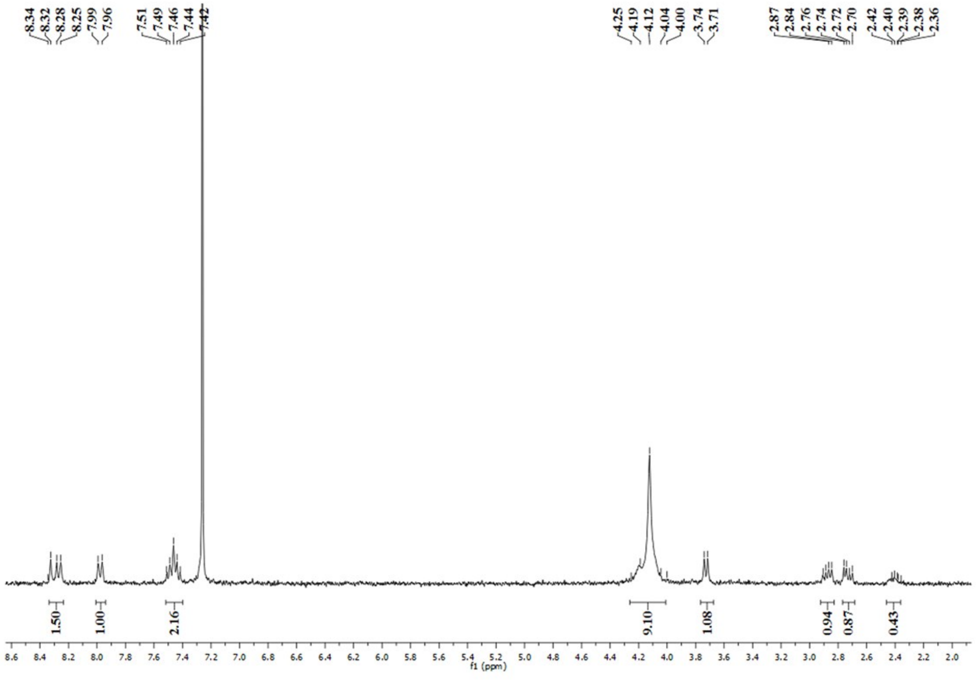


**Fig. S3:** $^{1}$H NMR spectrum of **L5,** $CDCl_3$, 298 K.

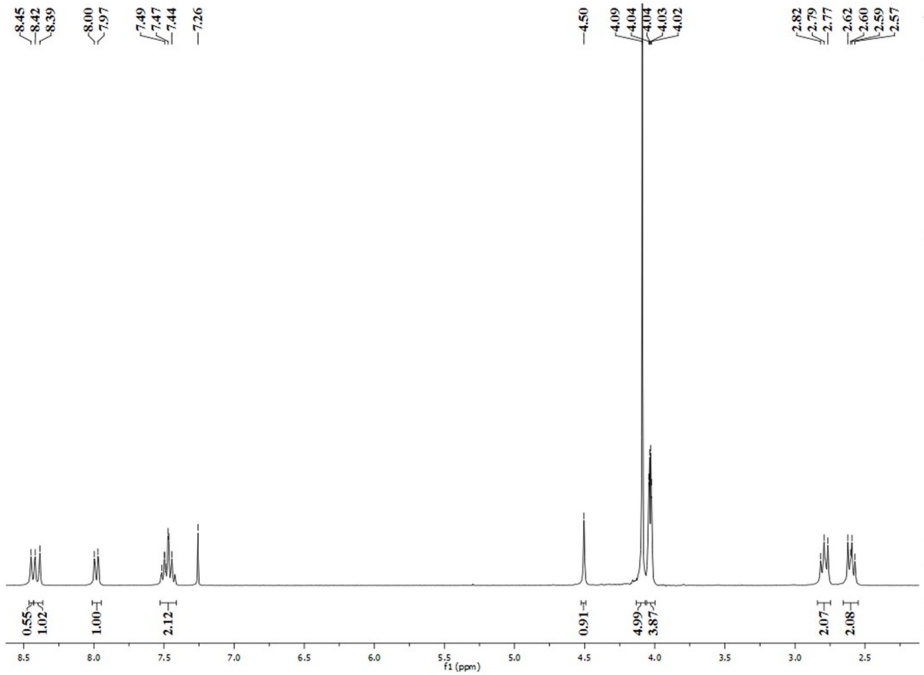


**Fig. S4:** MALDI-TOF Spectrum of **L3**

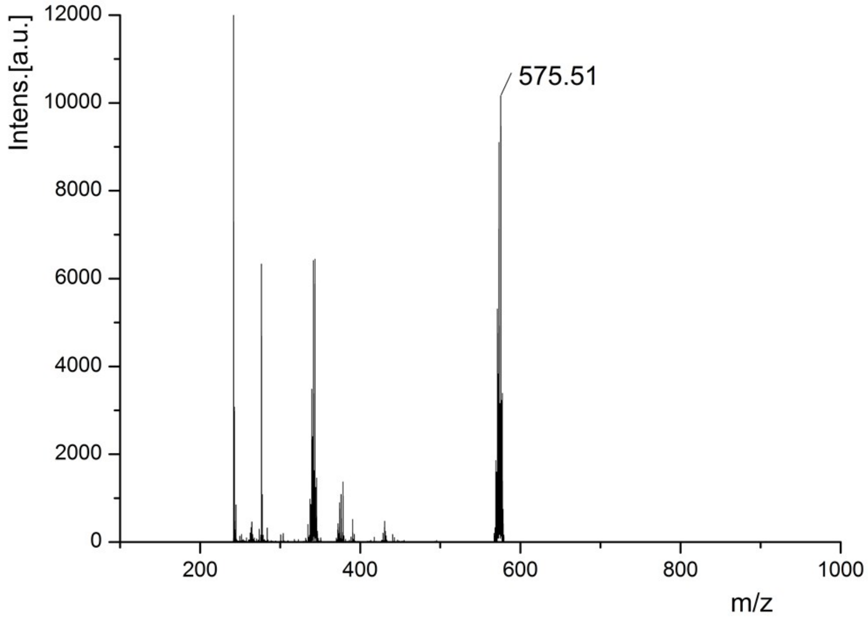


**Fig. S5:** MALDI-TOF Spectrum of **L4**

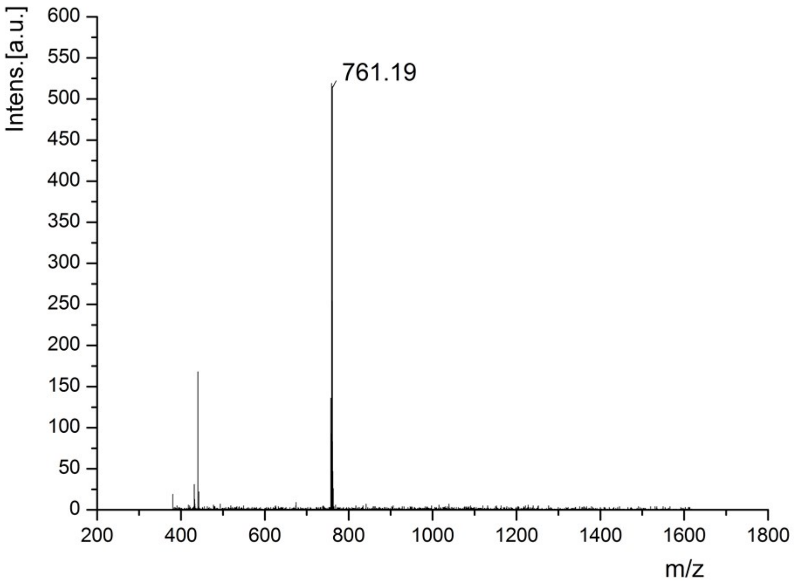


**Fig. S6:** ESI-MS spectrum of **L5**

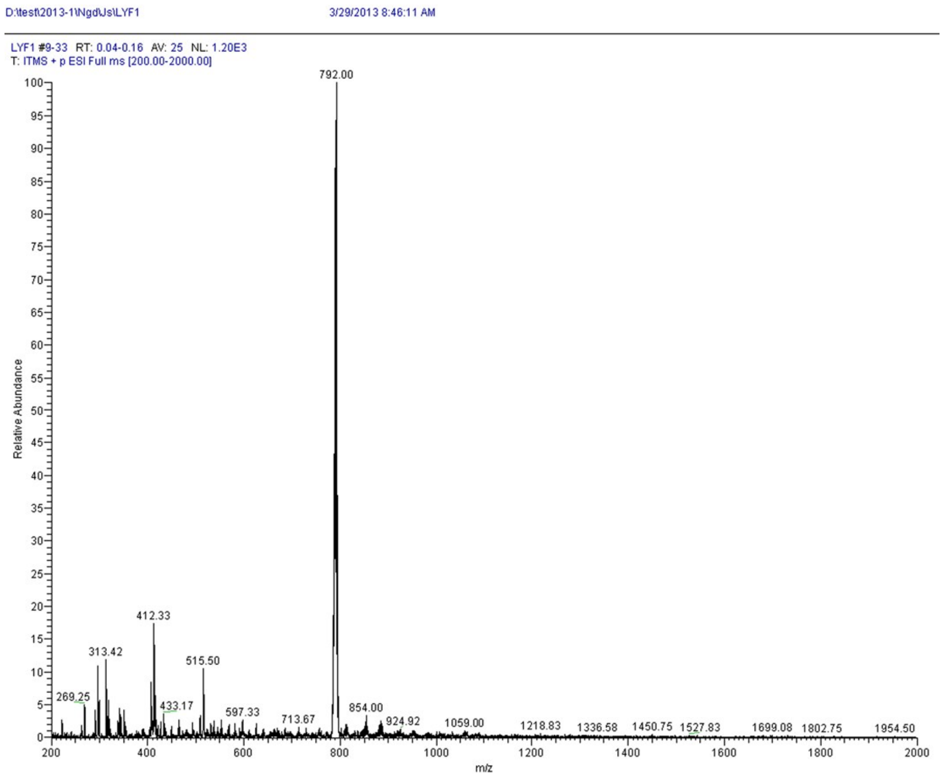


**Fig. S7:** Fluorescence spectra change of **L3** ($1 \times 10^{-4}$ M) in a $CH_2Cl_2$ solution upon addition of various metal ions.

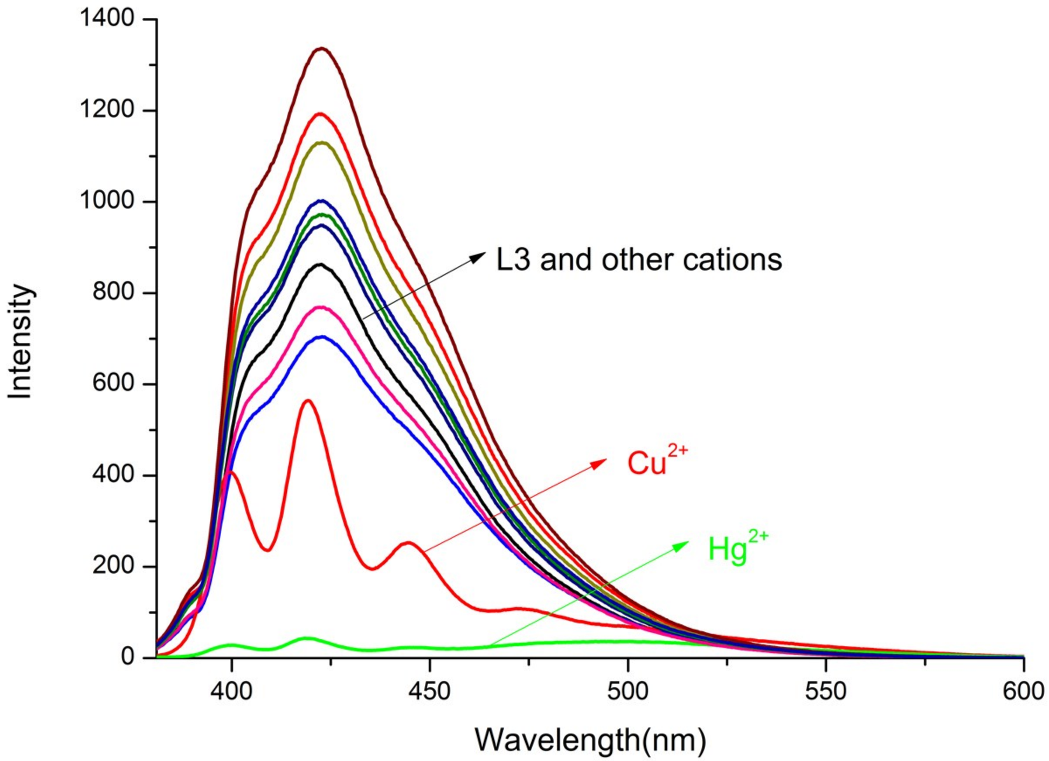


**Fig. S8:** Fluorescence spectra change of **L4** ($1 \times 10^{-4}$ M) in a $CH_2Cl_2$ solution upon addition of various metal ions

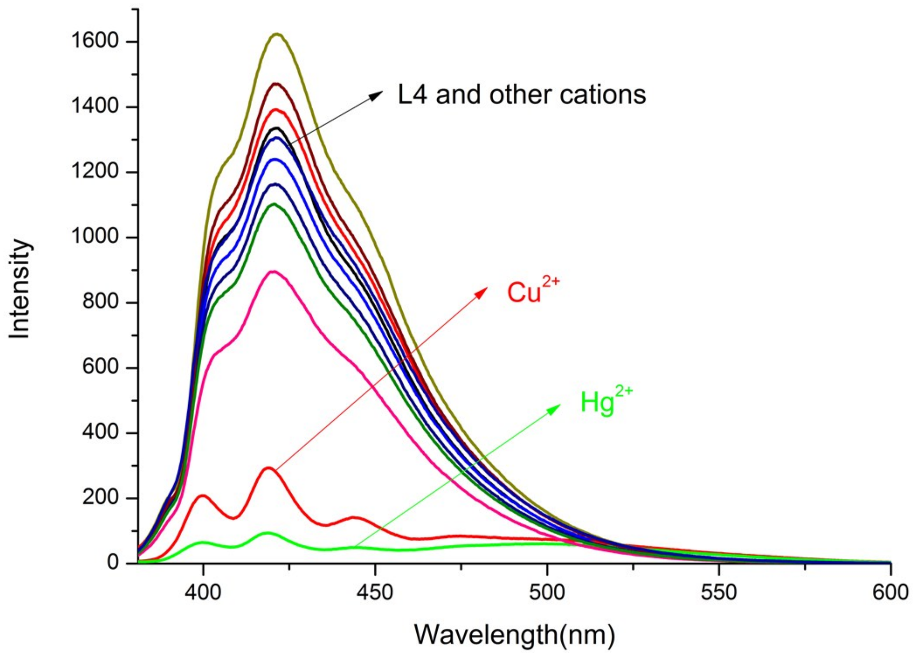


**Fig. S9:** UV/vis spectra changes of receptor **L3** ($1 \times 10^{-4}$ M) in a $CH_2Cl_2$ solution upon the addition of various metal ions.

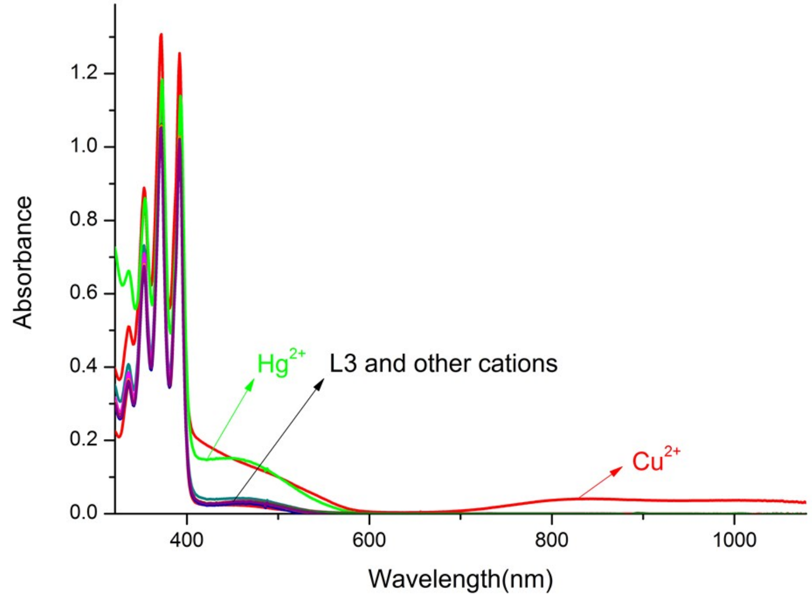


**Fig. S10:** UV/vis spectra changes of receptor **L4** ($1 \times 10^{-4}$ M) in a $CH_2Cl_2$ solution upon the addition of various metal ions.

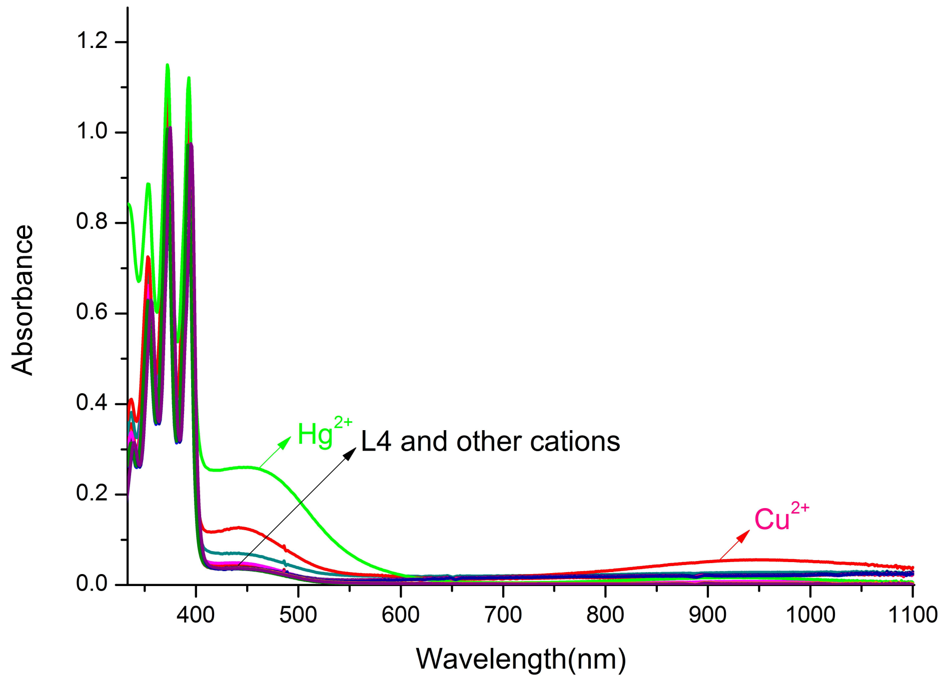


**Fig. S11:** UV/vis spectra changes of receptor **L5** ($1 \times 10^{-4}$ M) in a $CH_2Cl_2$ solution upon the addition of various metal ions.

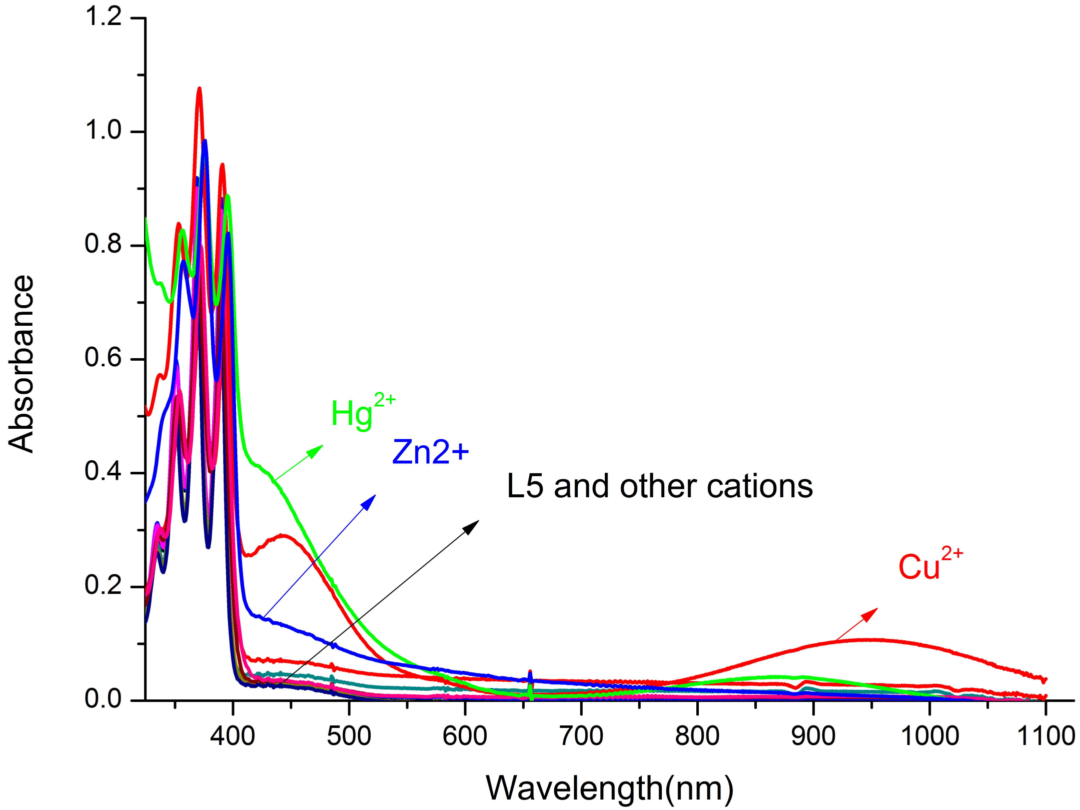


**Fig.S12:** Absorbance of **L5** at different concentrations of $Zn^{2+}$ added, normalized between the minimum absorbance and the maximum absorbance intensity. The detection limit was determined to be $6.62\times10^{-6}$ M.

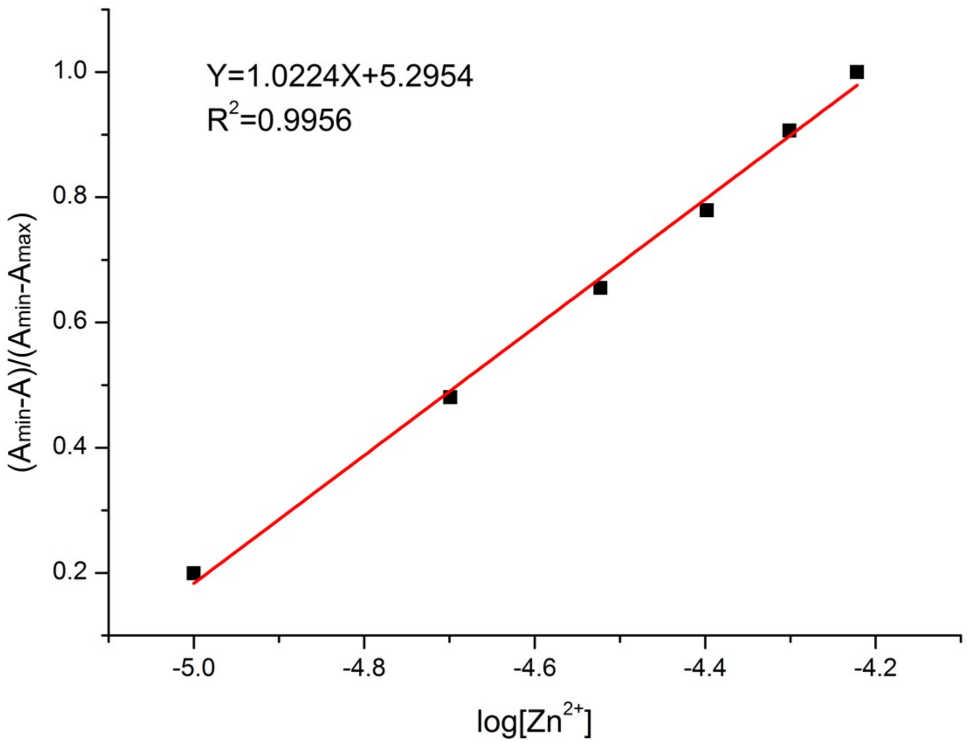
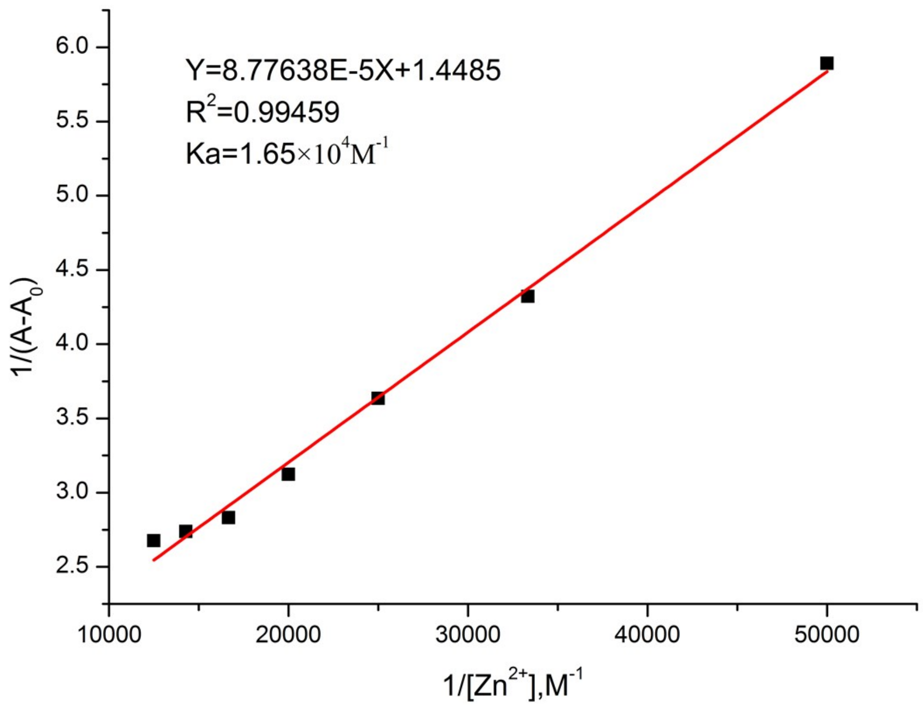


**Fig.S13:** Benesi-Hilderbrand plot of **L5** with $Zn(ClO_4)_2$.



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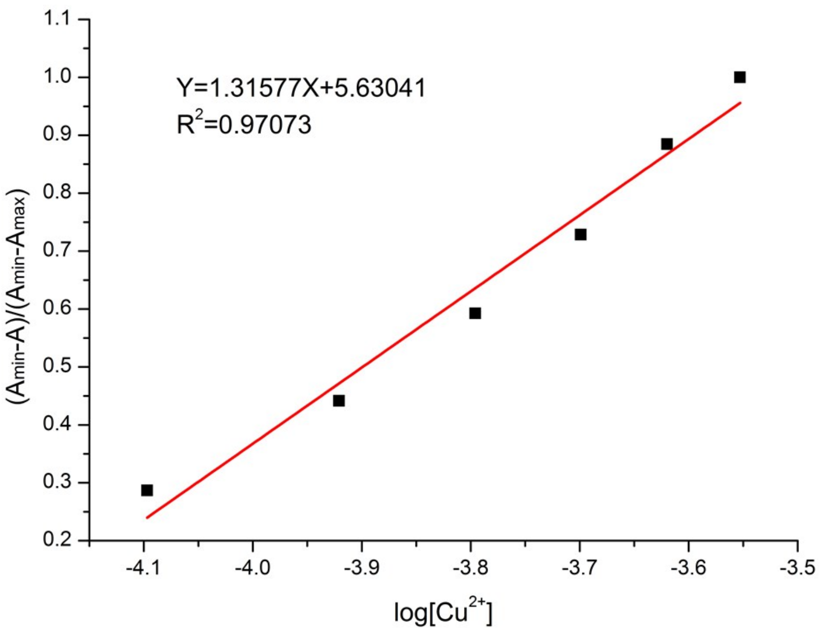

**Fig.S15:** Benesi-Hilderbrand plot of **L5** with $Cu(ClO_4)_2$.

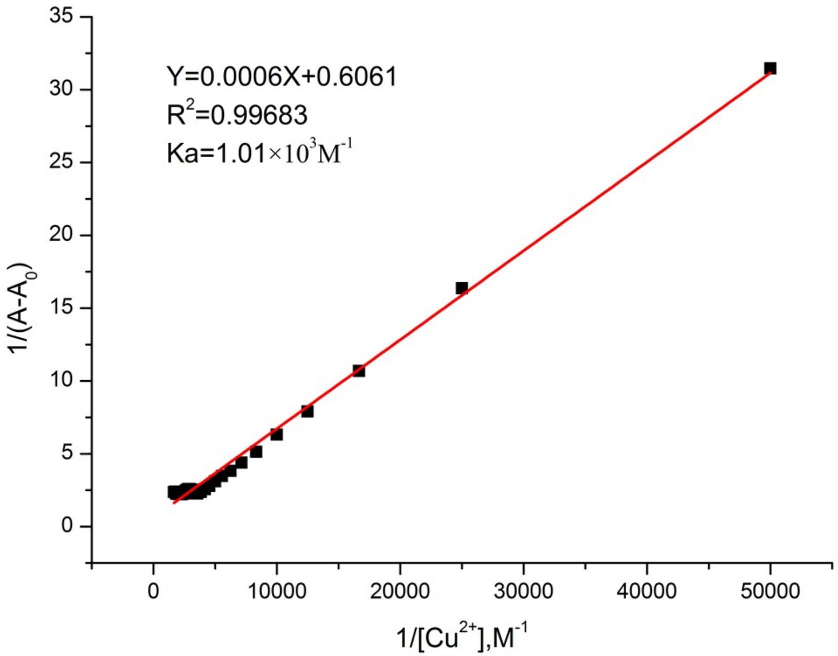

**Fig. S16:** Cyclic voltammogram of **L3** (black line) in $CH_3CN/CH_2Cl_2$ (1:1, v/v) solution upon addition of excess $Cu(ClO_4)_2$ (red line) and $Hg(ClO_4)_2$ (green line).

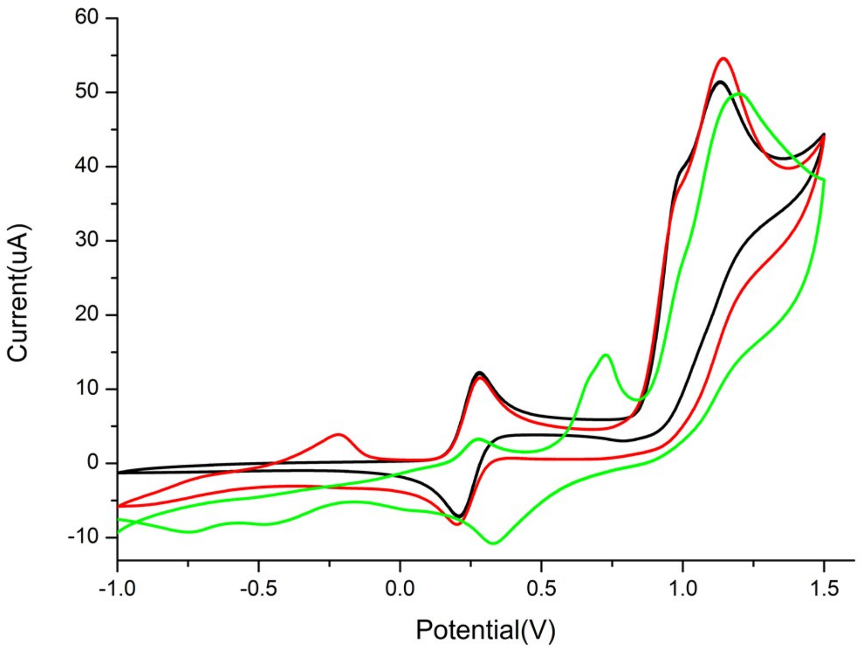


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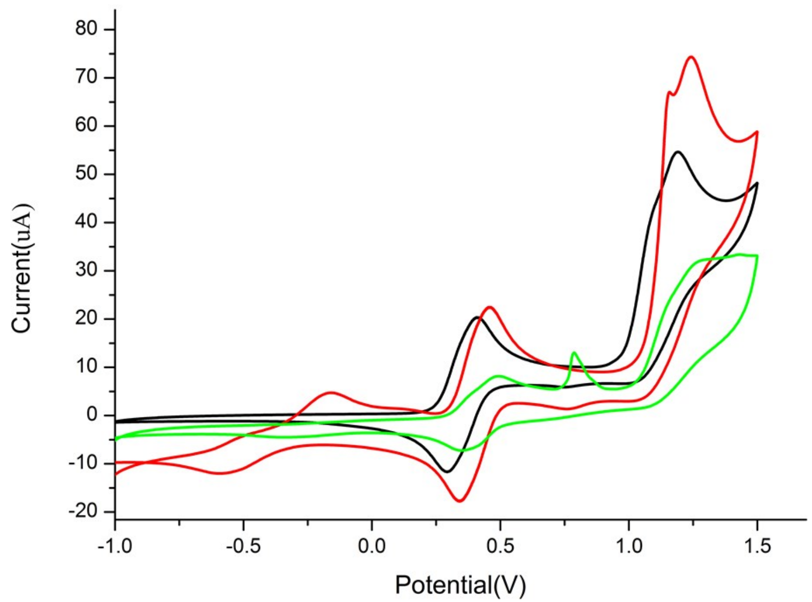
**Fig. S17:** Cyclic voltammogram of **L4** (black line) in $CH_3CN/CH_2Cl_2$ (1:1, v/v) solution upon addition of excess $Cu(ClO_4)_2$ (red line) and $Hg(ClO_4)_2$ (green line).



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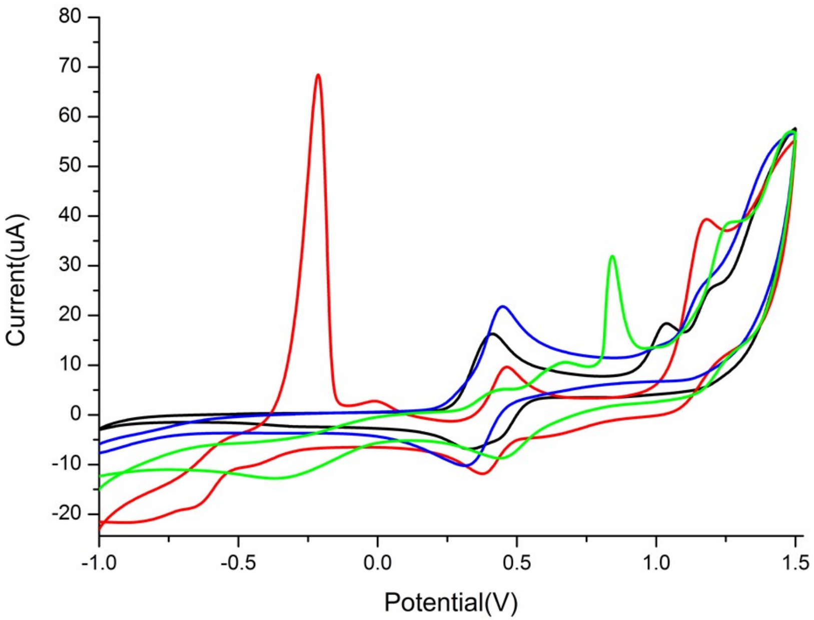

**Fig.S19:** IR spectrum of **L5**

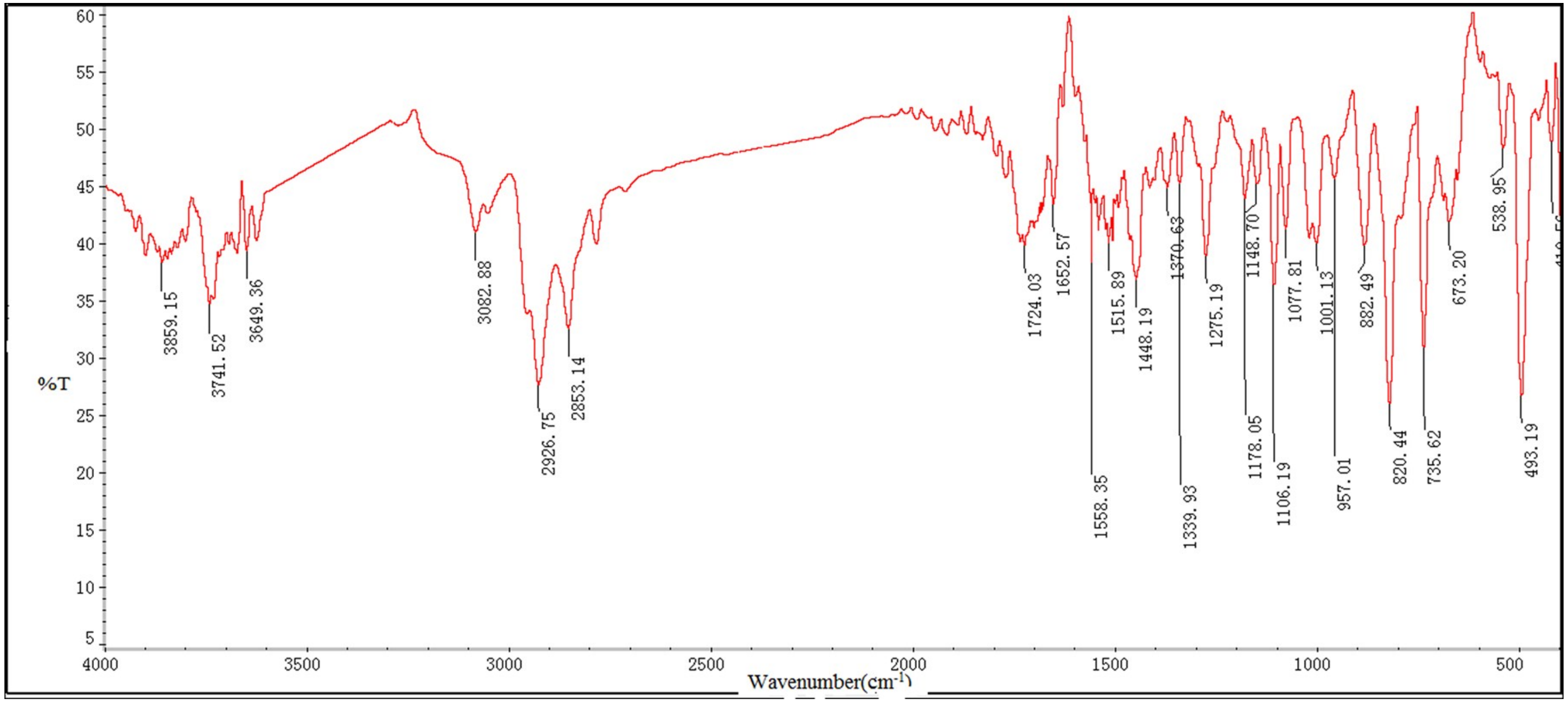

**Fig.S20:** IR spectrum of **L5** with excess $Cu(ClO_4)_2$

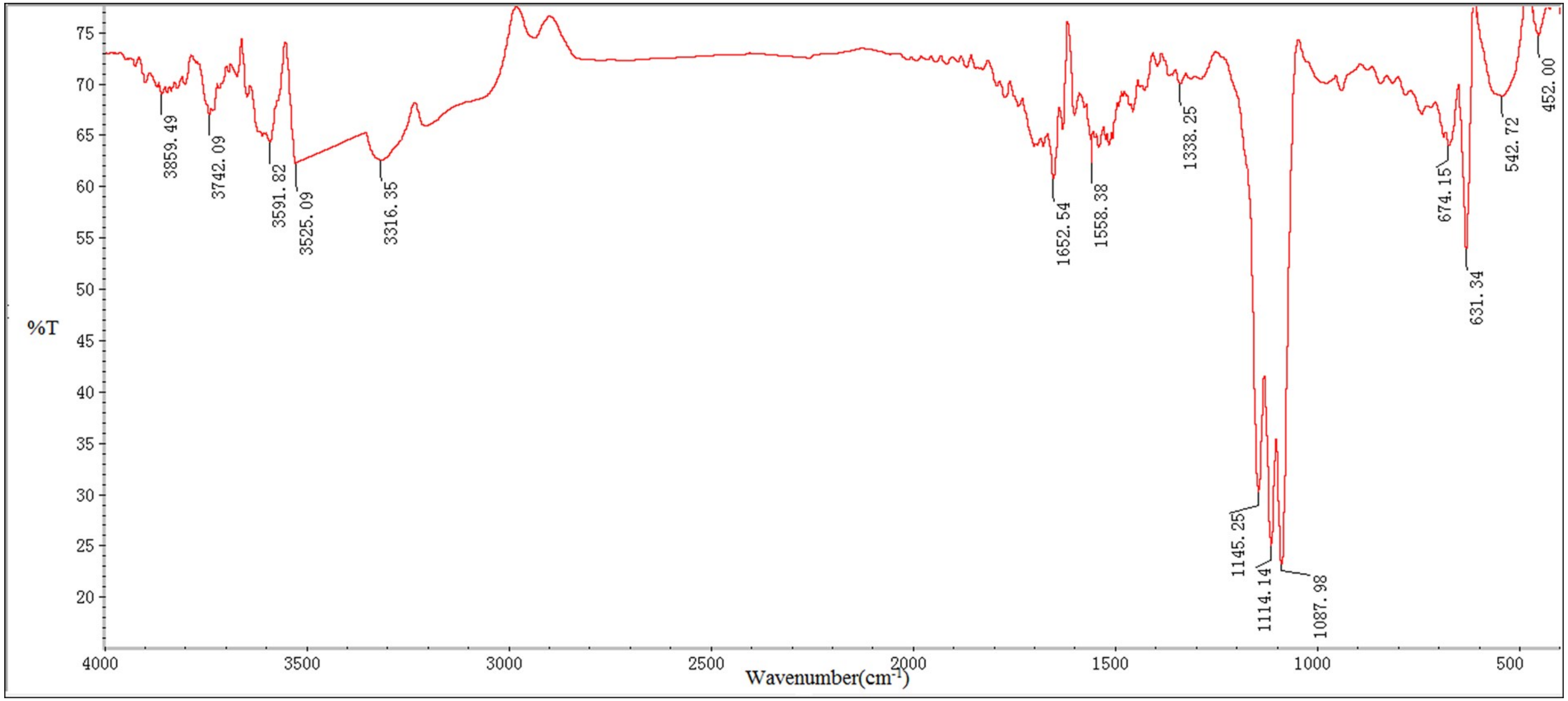

**Fig.S21:** IR spectrum of **L5** with excess $Zn(ClO_4)_2$

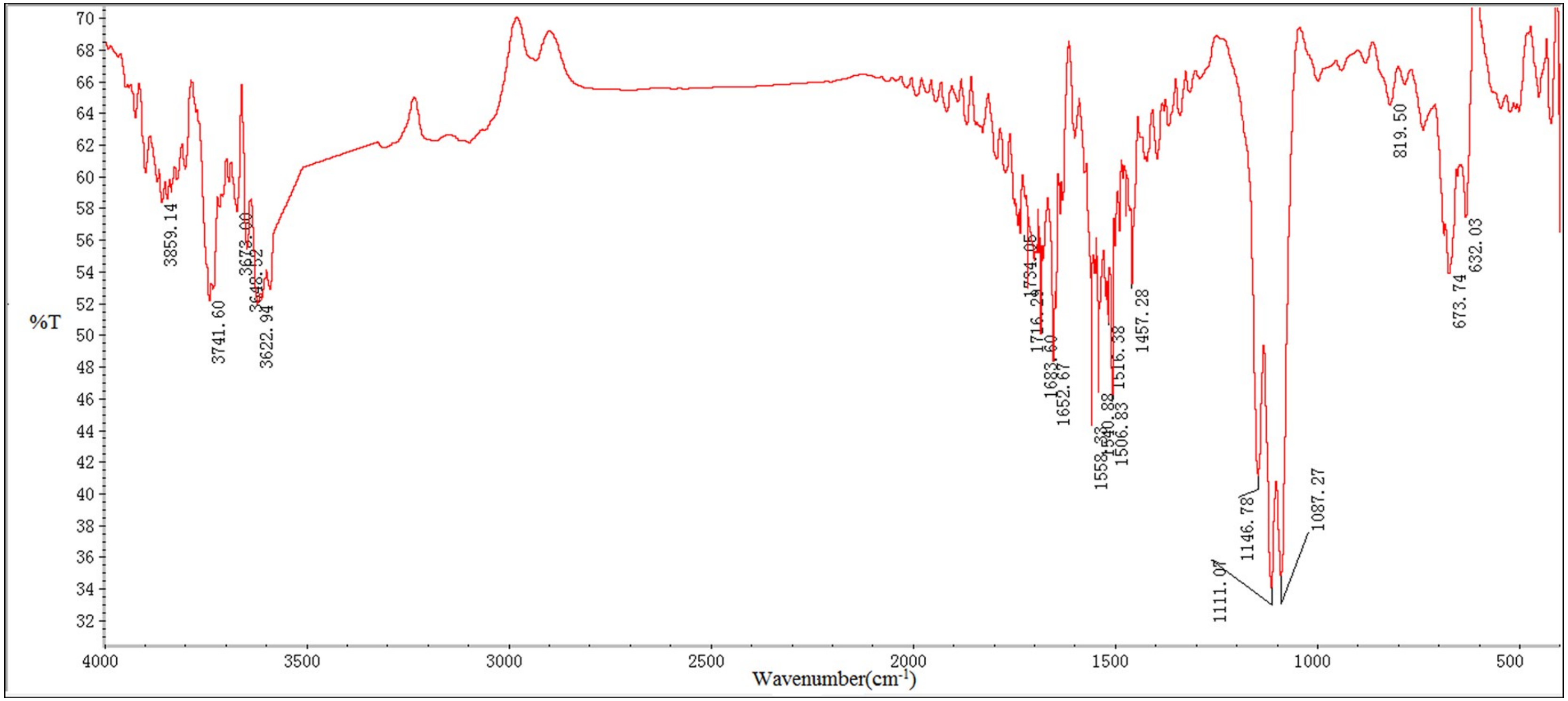

**Fig.S22:** IR spectrum of **L5** with excess $Hg(ClO_4)_2$

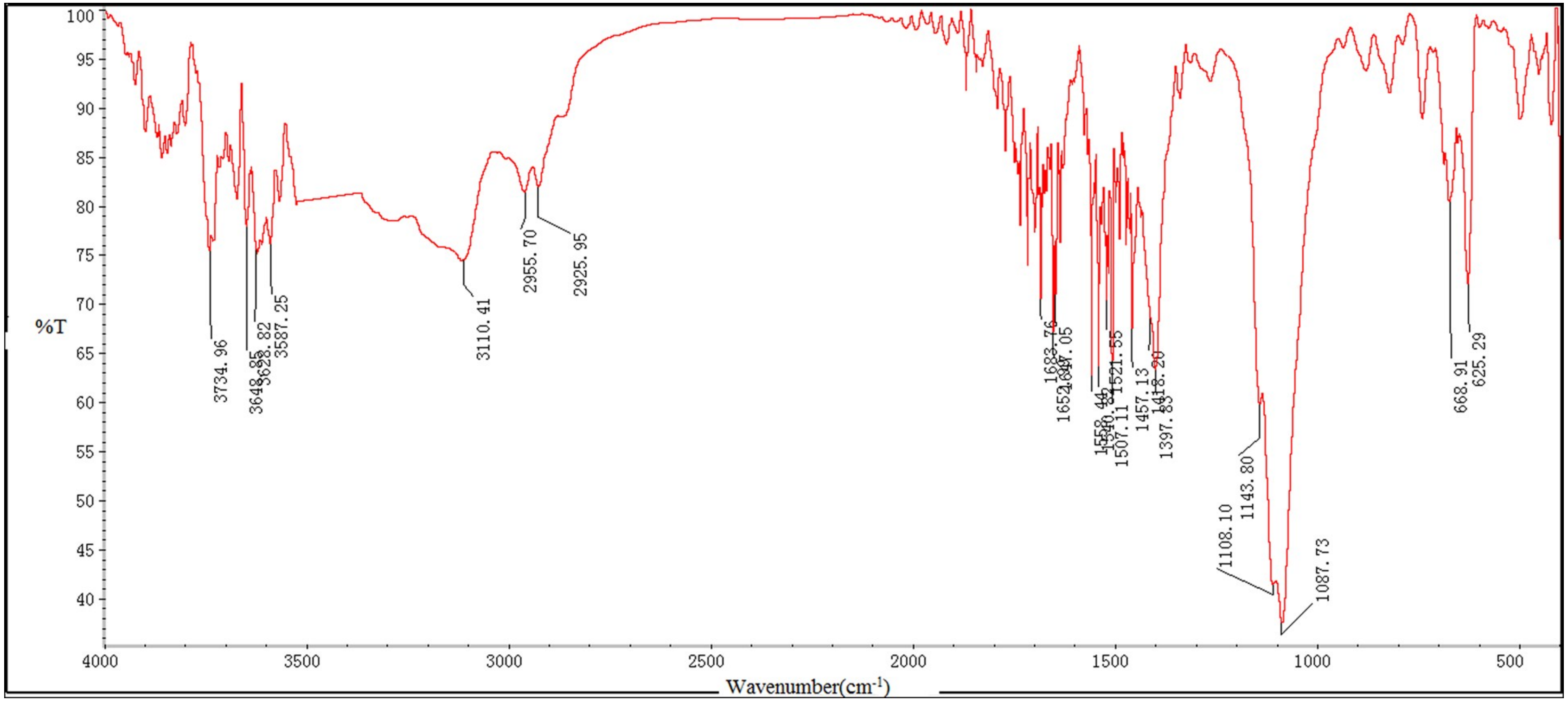

**Table S1:** Selected Bond Lengths (Å) and Bond Angles (°) for **L3-L5**

| **L3** | | **L4** | | **L5** | |
|---|---|---|---|---|---|
| Se1-C1 | 1.898(5) | Se1-C11 | 1.902(4) | Se1-C1 | 1.907(4) |
| Se1-C11 | 1.966(6) | Se1-C23 | 1.958(4) | Se1-C21 | 1.968(4) |
| Se2-C6 | 1.912(5) | Se2-C1 | 1.902(3) | Se2-C11 | 1.913(4) |
| Se2-C13 | 1.954(5) | Se2-C21 | 1.974(4) | Se2-C24 | 1.969(9) |
| | | | | N1-C25 | 1.463(4) |
| | | | | N1-C22 | 1.470(4) |
| | | | | N1-C23 | 1.478(4) |
| C1-Se1-C11 | 97.3(2) | C11-Se1-C23 | 100.53(2) | C1-Se1-C21 | 98.85(2) |
| C6-Se2-C13 | 104.4(2) | C1-Se2-C21 | 97.64(2) | C11-Se2-C24 | 94.45(2) |
| | | | | C25-N1-C22 | 110.8(3) |
| | | | | C25-N1-C23 | 111.4(3) |
| | | | | C22-N1-C23 | 113.8(3) |

**Table S2:** Selected Bond Lengths (Å) and Bond Angles (°) for **1-4**

| **1** | | **2** | | **3** | | **4** | |
|---|---|---|---|---|---|---|---|
| Se1-C1 | 1.904(4) | Se1-C1 | 1.896(4) | Se1-C1 | 1.906(1) | Se1-C18 | 1.888(7) |
| Se1-C11 | 1.967(4) | Se1-C11 | 1.984(5) | Se1-C11 | 1.962(1) | Se1-C17 | 1.975(6) |
| Se2-C6 | 1.915(4) | Se2-C6 | 1.902(5) | Se2-C6 | 1.914(9) | Se2-C30 | 1.878(7) |
| Se2-C27 | 1.962(4) | Se2-C27 | 1.971(5) | Se2-C13 | 1.967(1) | Se2-C29 | 1.964(7) |
| Cu-Cu#1 | 2.793(1) | Cu1-Cu1#1 | 2.782(1) | Cu1-Cu2 | 2.612(2) | Se1-Cu1 | 2.436(1) |
| Se1-Cu | 2.433(7) | Se1-Cu1 | 2.454(8) | Se1-Cu1 | 2.430(2) | Se2-Cu2#1 | 2.415(1) |
| Se2-Cu | 2.436(7) | Se2-Cu1 | 2.451(8) | Se2-Cu1 | 2.444(2) | Se3-Cu3 | 2.433(1) |
| Br-Cu | 2.452(7) | I1-Cu1 | 2.602(7) | Se3-Cu2 | 2.430(2) | Se4-Cu4#2 | 2.428(1) |
| Br-Cu#1 | 2.492(7) | I1-Cu1#1 | 2.627(8) | Se4-Cu2 | 2.433(2) | Cu2-Se2#1 | 2.415(1) |
| Cu-Br#1 | 2.492(7) | Cu1-I1#1 | 2.627(8) | I2-Cu1 | 2.566(2) | Cu4-Se4#2 | 2.428(1) |
| | | | | I2-Cu2 | 2.663(2) | Cu1-Cu3 | 2.768(2) |
| | | | | I1-Cu2 | 2.557(2) | Cu1-Cu4 | 2.886(2) |
| | | | | I1-Cu1 | 2.638(2) | Cu1-Cu2 | 2.811(2) |
| Se1-Cu-Se2 | 114.55(2) | Se2-Cu1-Se1 | 112.40(3) | Se1-Cu1-Se2 | 99.72(6) | Cu2-Cu3 | 2.788(2) |
| Se1-Cu-Br | 109.77(3) | Se1-Cu1-I1 | 105.49(3) | Se1-Cu1-I2 | 115.81(7) | Cu2-Cu4 | 2.752(1) |
| Se2-Cu-Br | 109.23(2) | Se2-Cu1-I1#1 | 103.24(3) | Se2-Cu1-I2 | 112.76(6) | Cu3-Cu4 | 2.893(2) |
| Se1-Cu-Br#1 | 109.86(3) | Se1-Cu1-I1#1 | 110.27(3) | Se1-Cu1-Cu2 | 129.31(8) | I1-Cu1 | 2.646(8) |
| Se2-Cu-Br#1 | 102.03(2) | Se2-Cu1-I1#1 | 103.24(3) | Se2-Cu1-Cu2 | 129.04(7) | I1-Cu2 | 2.656(1) |
| Br-Cu-Br#1 | 111.21(2) | I1-Cu1-I1#1 | 115.71(2) | I2-Cu1-Cu2 | 61.88(4) | I1-Cu3 | 2.705(1) |
| Se1-Cu-Cu#1 | 126.87(3) | Se1-Cu1-Cu1#1 | 125.23(4) | Se1-Cu1-I1 | 100.35(6) | I2-Cu4 | 2.653(1) |
| Se2-Cu-Cu#1 | 118.37(3) | Se2-Cu1-Cu1#1 | 122.35(3) | Se2-Cu1-I1 | 105.43(6) | I2-Cu1 | 2.691(1) |
| Br-Cu-Cu#1 | 56.27(2) | I1-Cu1-Cu1#1 | 58.30(2) | I2-Cu1-I1 | 120.14(6) | I2-Cu2 | 2.777(9) |
| Br#1-Cu-Cu#1 | 54.94(2) | I1#1-Cu1-Cu1#1 | 57.41(2) | Cu2-Cu1-I1 | 58.29(4) | I3-Cu2 | 2.601(1) |
| | | | | Se3-Cu2-Se4 | 99.34(6) | I3-Cu3 | 2.698(1) |
| | | | | Se3-Cu2-I1 | 116.87(7) | I3-Cu4 | 2.770(9) |
| | | | | Se4-Cu2-I1 | 115.09(7) | I4-Cu3 | 2.631(8) |
| | | | | Se3-Cu2-Cu1 | 129.65(7) | I4-Cu4 | 2.680(1) |
| | | | | Se4-Cu2-Cu1 | 128.16(7) | I4-Cu1 | 2.697(1) |
| | | | | I1-Cu2-Cu1 | 61.36(4) | Se1-Cu1-I1 | 110.34(4) |
| | | | | Se3-Cu2-I2 | 102.47(6) | Se1-Cu1-I2 | 102.11(3) |
| | | | | Se4-Cu2-I2 | 100.35(6) | I1-Cu1-I2 | 111.83(3) |

| | | | | | |
|---|---|---|---|---|---|
| | | I1-Cu2-I2 | 119.54(6) | Se1-Cu1-I4 | 110.88(4) |
| | | Cu1-Cu2-I2 | 58.21(4) | I1-Cu1-I4 | 113.79(3) |
| | | | | I2-Cu1-I4 | 107.24(3) |
| | | | | Se2#1-Cu2-I3 | 114.01(4) |
| | | | | Se2#1-Cu2-I1 | 109.93(4) |
| | | | | I3-Cu2-I1 | 111.85(3) |
| | | | | Se2#1-Cu2-I2 | 95.42(3) |
| | | | | I3-Cu2-I2 | 115.59(3) |
| | | | | I1-Cu2-I2 | 108.88(3) |
| | | | | Se3-Cu3-I4 | 112.80(4) |
| | | | | Se3-Cu3-I3 | 100.81(3) |
| | | | | I4-Cu3-I3 | 111.04(3) |
| | | | | Se3-Cu3-I1 | 109.89(3) |
| | | | | I4-Cu3-I1 | 113.99(3) |
| | | | | I3-Cu3-I1 | 107.39(3) |
| | | | | Se4#2-Cu4-I2 | 112.31(4) |
| | | | | Se4#2-Cu4-I4 | 109.24(4) |
| | | | | I2-Cu4-I4 | 108.88(3) |
| | | | | Se4#2-Cu4-I3 | 104.63(4) |
| | | | | I2-Cu4-I3 | 114.12(3) |
| | | | | I4-Cu4-I3 | 107.43(3) |