Supplementary Material (ESI) for Dalton Transactions

Ferrocene substitution in amino acid strengthens the axial binding in Cu(II) complexes and separates the hydrophobic and hydrophilic region in the Crystals

Subash Chandra Sahoo and Manabendra Ray*

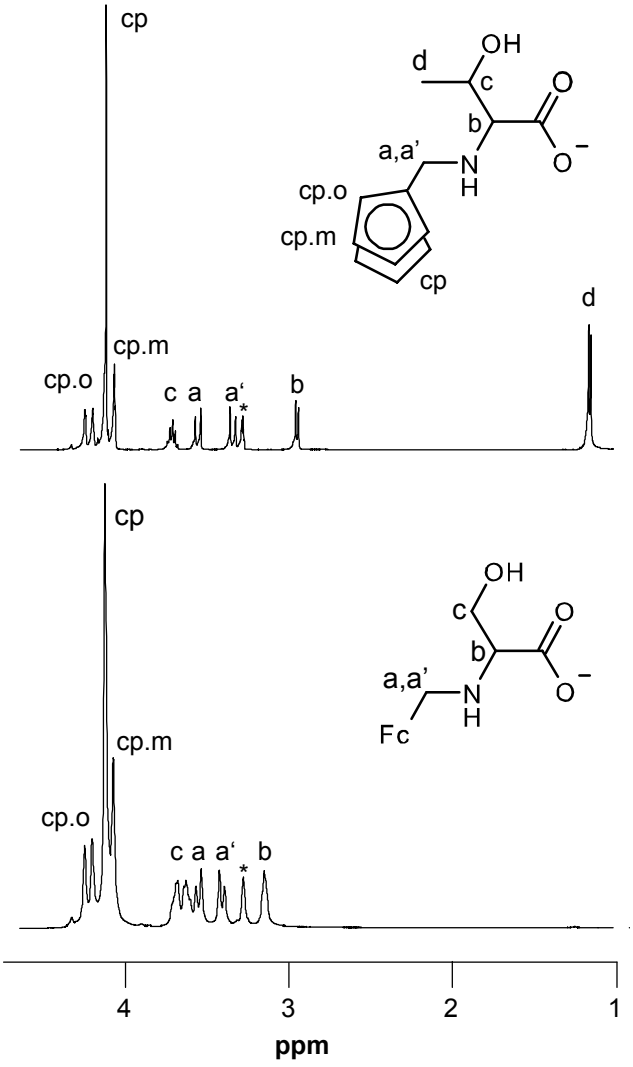

Figure S1. NMR spectra of **4** and **3** in CD_3OD with 1eq. of LiOH.

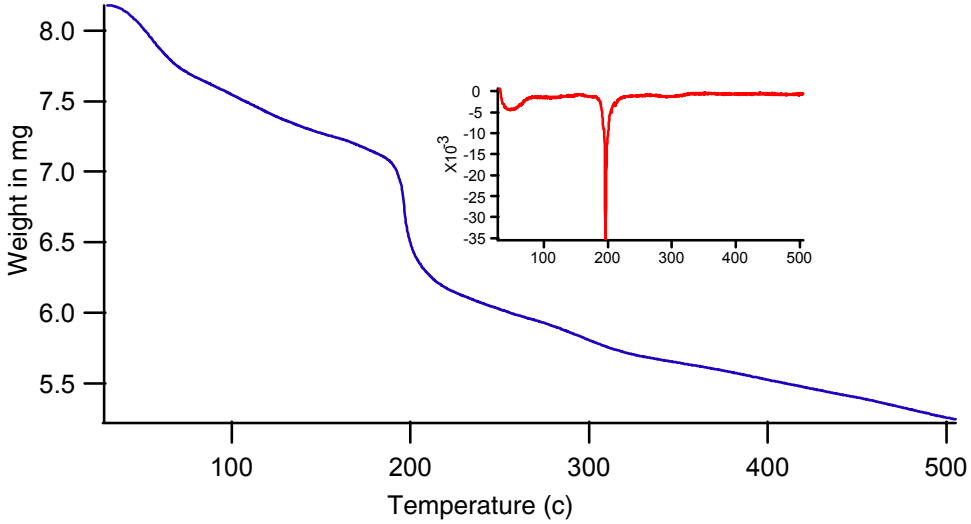

Figure S2. TGA plot of **2a** with derivative (DTA) plot of TGA as inset.

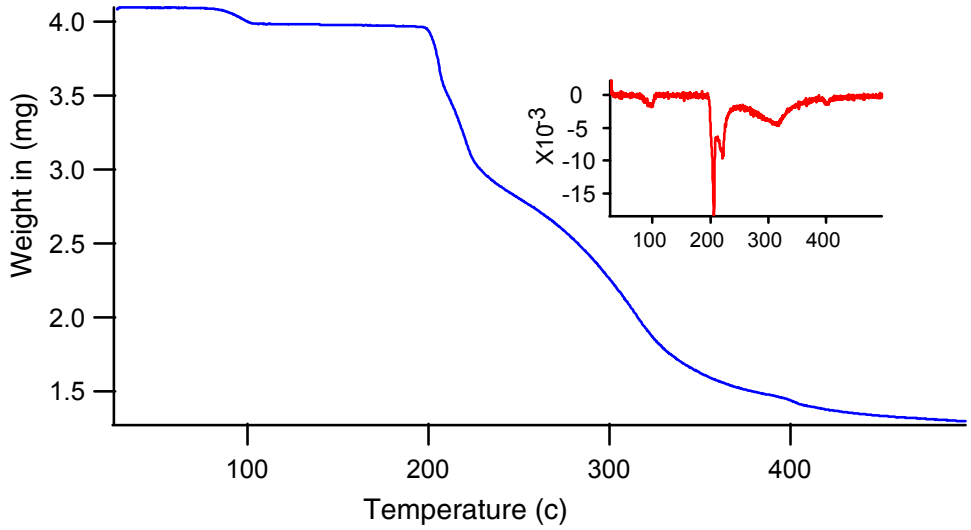

Figure S3. TGA plot of **3a** with derivative (DTA) plot of TGA as inset.

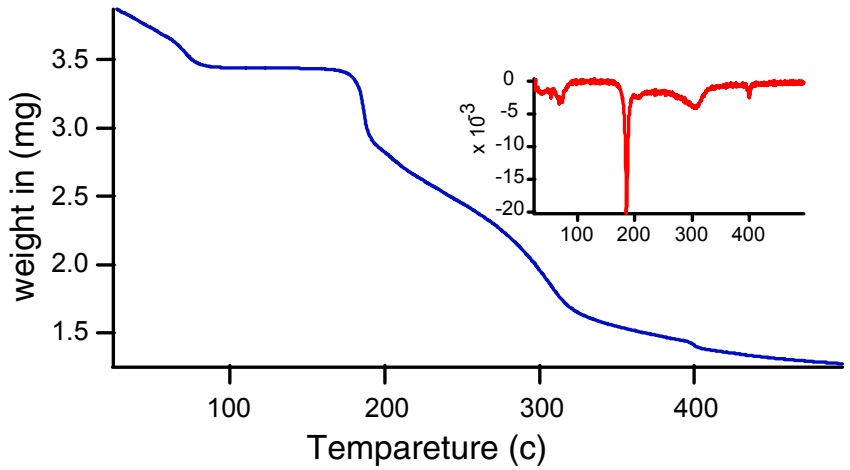

Figure S4. TGA plot of **4a** with derivative (DTA) plot of TGA as inset.

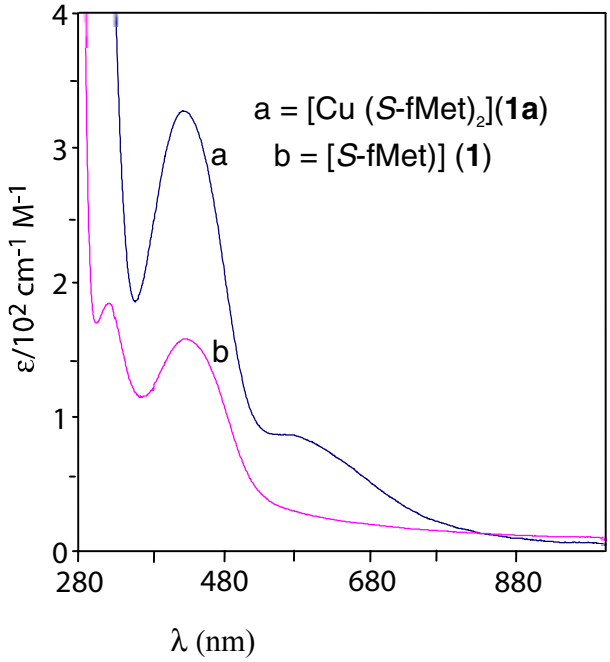

Figure S5. The UV-vis spectra of **1a** in MeOH and **1** in MeOH & LiOH.

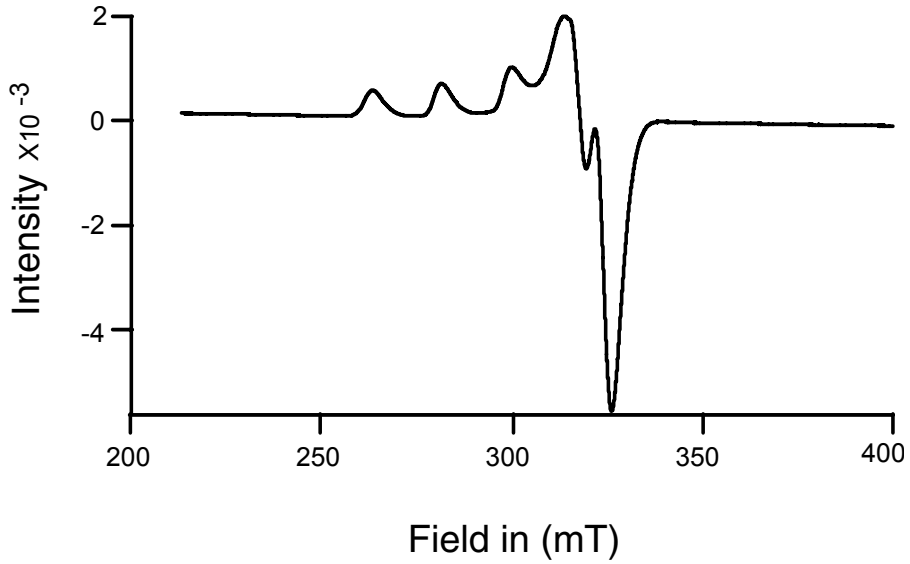

Figure S6. EPR of **1a** in MeOH at 77k.

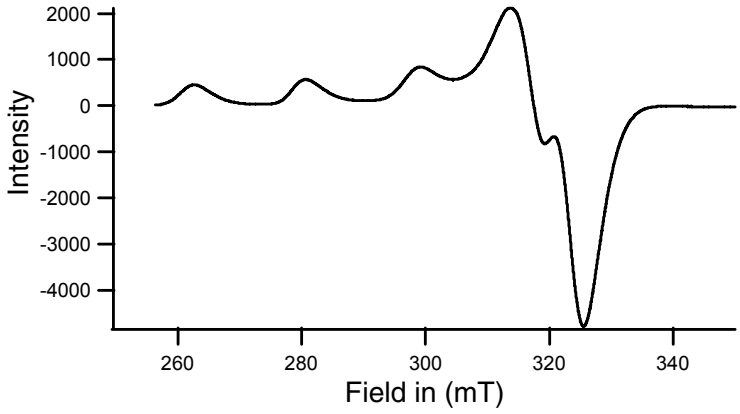

Figure S7. EPR of **3a** in MeOH at 77k.

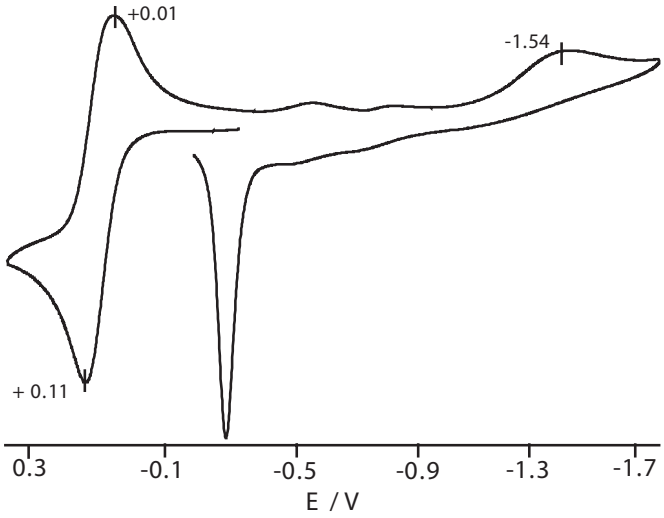

Figure S8. Cyclic Voltammogram of **1a** in DMF.
Condition: Scan rate 50 mV S^{-1}.glassy carbon working electrode. Supporting electrolyte Tetrabutylammonium perchlorate. Potentials shown are vs Fc^{+}/Fc.

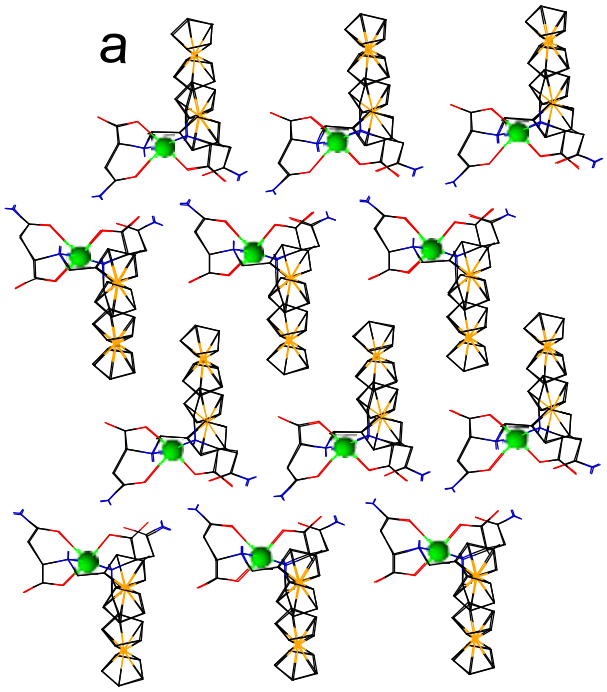

Figure S9. Alternative layers of hydrophilic and hydrophobic regions in **2a**.

Table S1. Selected Bond Lengths (Å) and angles (º) for **1a, 2a, 3a, 4a** and their amino acid analogue**.**

	1a	Cu(L-meth)$_2$	**2a**	Cu(L-asn)$_2$	**3a**	Cu(L-ser)$_2$	**4a**	Cu(L-thr)$_2$
Cu-N1	2.0188(15)	1.97(1)	1.985(5)	2.004(28)	2.0172(16)	1.988(6)	2.014(3)	1.968(8)
Cu-N1A	2.0288(16)	2.01(1)	2.003(5)	2.035(26)	2.0172(16)	1.975(6)	2.009(3)	1.982(8)
Cu-O1	1.9406(15)	1.970(8)	1.927(5)	1.947(21)	1.9206(15)	1.970(6)	1.946(3)	1.941(7)
Cu-O1A	1.9194(14)	1.944(8)	1.923(4)	1.954(22)	1.9275(15)	1.952(6)	1.937(3)	1.957(7
Cu-axial	2.7906(6)	2.751(7)	2.414(5)	2.529(20)	2.3876(17)	2.359(6)	2.258(4)	2.478(8)
	Cu-S	Cu-O_{carbo}					Cu-O_{water}	Cu-O_{carbo}
N1-Cu-O1A	94.22(6)	95.9(4)	96.8(2)	96.1(10)	92.14(6)	82.4(2)	96.47(13)	96.4(3)
O1A-Cu-N1A	85.05(6)	84.2(4)	83.94(19)	82.4(9)	85.61(7)	88.3(2)	85.00(12)	83.4(3)
N1A-Cu-O1	95.02(6)	96.3(4)	97.2(2)	94.5(10)	95.62(7)	83.9(2)	92.46(12)	96.2(3)
O1-Cu-N1	84.28(6)	83.7(4)	83.4(2)	86.9(10)	85.40(7)	105.0(2)	84.37(12)	83.6(3)
N1-Cu-axial	86.34(4)	89.3(3)	82.76(19)	94.6(9)	99.56(7)		99.50(13)	93.2(3)
axial-Cu-O1	91.70(5)	85.0(3)	86.92(19)	93.5(8)	87.57(6)		91.67(14)	89.7(3)
O1-Cu-O1A	174.48(6)	179.6(4)	174.6(2)	176.2(10)	173.83(7)	170.7(2)	174.49(13)	177.5(3)
N1-Cu-N1A	164.99(6)	175.0(3)	166.7(2)	175.3(10)	167.93(7)	172.2(2)	161.30(13)	172.1(3)
		Ref. 3(d)		Ref. 3(c)		Ref.3(b)		Ref. 3(f)