Supplementary figures and tables DT paper (NCH)

1. ESI Table S1.1 and S1.2 (Crystallographic data and selected bond lengths and angles of **1**)

ESI Tables S1.1

Compound	**1** [Cu(phen)(L-ser)(H_2O)]NO_3
Empirical formula	C_{15} H_{16} Cu N_4 O_7
Formula weight	427.86
Crystal system	Triclinic
Crystal size (mm)	0.34 x 0.34 x 0.38
Color	Blue
Shape	Block
Space group	*P*1 (No.1)
Unit cell dimensions (Å),(°)	*a* = 7.4893(3) α = 97.4994(16) *b* = 9.7967(4) β = 106.9521(16) *c* = 12.1077(5) γ = 107.5688(16)
Volume, (Å^3)	786.51(6)
Z	2
ρ_{calc} (g cm^{-3})	1.807
Mμ (mm^{-1})	1.441
F (000)	438
Theta range for collection (°)	2.53 – 27.18
Radiation (MoKα) (Å)	0.71073
Limiting Frequency	-9 ≤ h ≤ 9 -11 ≤ k ≤ 12 -14 ≤ l ≤ 15
Total reflections	11008
Independent reflections	5396
Refinement method	Full matrix least-squares refinement on F^2
Data/restraints/parameters	5396/471/491
Goodness of fit	1.072
Final R indices [I>2 σ (I)]	4.01%
R indices (all data)	9.91%
Largest diff. peak & hole (e Å^3)	0.424 and -0.525

ESI Tables S1.2

Bond Distances (Angstrom)			
Cu1-O1	1.934(5)	C5-C6	1.350(8)
Cu1-O7	2.275(4)	O6-C18	1.419(7)
Cu1-N1	1.998(5)	C6-C7	1.414(8)
Cu1-N2	2.027(5)	C7-C15	1.406(8)
Cu1-N3	2.013(5)	C7-C8	1.439(9)
Cu2-O4	1.938(4)	C8-C9	1.374(8)
Cu2-O8	2.265(4)	C9-C10	1.422(8)
Cu2-N4	1.998(5)	C10-C11	1.414(8)
Cu2-N5	2.018(5)	C10-C14	1.430(8)
Cu2-N6	2.005(5)	C11-C12	1.358(8)
O1-C1	1.286(7)	C12-C13	1.399(9)
O2-C1	1.232(6)	C14-C15	1.417(8)
O3-C3	1.431(6)	N4-C17	1.494(6)
N1-C2	1.483(6)	N2-C4	1.312(8)
N2-C15	1.374(8)	N3-C13	1.316(8)
N5-C30	1.355(8)	N3-C14	1.348(7)
N5-C19	1.338(8)	C1-C2	1.540(6)
N6-C29	1.370(7)	N6-C28	1.343(8)
C2-C3	1.516(6)	C25-C26	1.415(8)
O4-C16	1.271(7)	C26-C27	1.385(8)
C4-C5	1.411(9)	C27-C28	1.411(8)
O5-C16	1.239(6)	C29-C30	1.451(8)
O9-N7	1.242(7)	O10-N7	1.253(7)
O11-N7	1.255(7)	C16-C17	1.535(6)
C17-C18	1.511(6)	C19-C20	1.392(9)
C20-C21	1.386(8)	C21-C22	1.408(9)
C22-C30	1.395(8)	C22-C23	1.438(9)
C23-C24	1.351(8)	O12-N8	1.265(6)
C24-C25	1.446(8)	O13-N8	1.254(7)

C25-C29	1.368(8)	O14-N8	1.253(7)

Bond Angles	(Degrees)		
O1-Cu1-O7	96.64(17)	C3-O3-H3	109.00
O1-Cu1-N1	84.4(2)	O1-Cu1-N2	165.6(2)
O1-Cu1-N3	91.13(19)	O7-Cu1-N1	96.23(18)
O7-Cu1-N2	96.53(18)	O2-C1-C2	118.7(4)
O7-Cu1-N3	93.09(18)	N1-Cu1-N2	100.0(2)
N1-Cu1-N3	170.1(2)	O1-C1-C2	116.6(4)
N2-Cu1-N3	82.33(19)	O4-Cu2-N5	166.03(19)
O4-Cu2-N6	91.07(19)	O1-C1-O2	124.7(5)
O8-Cu2-N4	96.65(18)	N1-C2-C1	109.0(3)
O8-Cu2-N5	95.98(18)	N1-C2-C3	113.3(4)
O8-Cu2-N6	93.34(18)	C1-C2-C3	111.4(4)
O4-Cu2-O8	96.32(17)	O3-C3-C2	108.7(4)
O4-Cu2-N4	85.1(2)	N2-C4-C5	121.6(6)
N5-Cu2-N6	81.63(19)	Cu2-O4-C16	116.3(3)
N4-Cu2-N5	100.0(2)	C4-C5-C6	120.8(6)
N4-Cu2-N6	169.6(2)	C5-C6-C7	119.0(5)
Cu1-O1-C1	114.6(4)	C6-C7-C15	117.3(5)
Cu1-N1-C2	106.6(3)	C6-C7-C8	124.1(5)
Cu1-N2-C4	129.8(4)	C8-C7-C15	118.6(5)
Cu1-N2-C15	111.4(4)	C7-C8-C9	120.4(6)
C4-N2-C15	118.8(5)	C8-C9-C10	121.6(6)
Cu1-N3-C13	128.7(4)	C9-C10-C14	118.9(5)
Cu1-N3-C14	111.9(4)	C11-C10-C14	115.8(5)
C13-N3-C14	119.3(5)	C9-C10-C11	125.3(5)
C10-C11-C12	120.0(5)	Cu2-N6-C29	114.1(4)
C11-C12-C13	120.0(6)	C28-N6-C29	117.9(5)
N3-C13-C12	122.0(6)	N3-C14-C15	118.0(5)
C10-C14-C15	119.2(5)	N3-C14-C10	122.7(5)

C7-C15-C14	121.3(5)	N2-C15-C14	116.3(5)
N2-C15-C7	122.4(5)	Cu2-N4-C17	109.5(3)
Cu2-N5-C30	113.0(4)	C19-N5-C30	117.4(5)
O4-C16-O5	124.8(5)	Cu2-N5-C19	129.6(4)
O4-C16-C17	117.2(4)	O5-C16-C17	118.0(4)
C16-C17-C18	111.5(3)	N4-C17-C18	110.7(4)
N4-C17-C16	110.1(4)	Cu2-N6-C28	128.0(4)
O6-C18-C17	111.9(4)	N5-C19-C20	122.8(6)
C19-C20-C21	119.1(5)	C20-C21-C22	120.0(5)
C21-C22-C30	116.1(5)	C21-C22-C23	124.6(5)
C23-C22-C30	119.4(6)	C22-C23-C24	121.3(6)
C23-C24-C25	120.5(6)	C24-C25-C26	123.2(5)
C26-C25-C29	117.9(5)	C24-C25-C29	118.8(5)
C25-C26-C27	118.8(5)	C26-C27-C28	119.7(5)
N6-C28-C27	121.6(5)	N6-C29-C30	114.4(5)
C25-C29-C30	121.5(5)	N6-C29-C25	124.1(5)
C22-C30-C29	118.4(5)	N5-C30-C22	124.8(5)
N5-C30-C29	116.8(5)	O9-N7-O11	121.4(5)
O10-N7-O11	120.3(5)	O9-N7-O10	118.3(5)
O12-N8-O13	120.2(5)	O12-N8-O14	119.4(5)
O13-N8-O14	120.4(5)		

2. ESI Tables S2.1 and S2.2 (Crystallographic data and selected bond lengths and angles of **3**)

ESI Tables S2.1

Compound	**3** L-[Cu(phen)(OCA)(H_2O)]NO_3·H_2O
Empirical formula	C_{16} H_{18} Cu N_4 O_8
Formula weight	457.88
Crystal system	orthorhombic
Crystal size (mm)	0.08 x 0.10 x 0.40
Color	Blue
Shape	Needle
Space group	$P2_12_12_1$ (No.19)
Unit cell dimensions (Å),(°)	*a* = 6.6836(3) α = 90.00
	b = 12.2756(4) β = 90.00
	c = 21.8809(8) γ = 90.00
Volume, (Å^3)	1795.22(12)
Z	4
ρ_{calc} (g cm^{-3})	1.694
Mμ (mm^{-1})	1.273
F (000)	940
Temperature (K)	103
Theta range for collection (°)	2.49 – 28.91
Radiation (MoKα) (Å)	0.71073
Limiting frequency	-9 ≤ h ≤ 9
	0 ≤ k ≤ 17
	0 ≤ l ≤ 31
Total reflections	19885
Independent reflections	5710 [R(int) = 3.93%]
Refinement method	Full matrix least-squares refinement on F^2
Data/restraints/parameters	5708/6/277
Goodness of fit	1.021
Final R indices [I>2 σ (I)]	6955 [4.988° < 2θ < 57.82°]
R indices (all data)	R1 = 3.16%, wR2 = 9.26%
Largest diff. peak & hole (e Å^3)	0.601 and 0.649

ESI Tables S2.2

Bond Distances (Å)			
Cu1-O1	1.9464(13)	C7-C8	1.411(2)
Cu1-O4	2.2805(14)	C8-C16	1.406(2)
Cu1-N1	2.0001(15)	C8-C9	1.433(2)
Cu1-N2	2.0253(14)	C9-C10	1.356(2)
Cu1-N3	1.9826(13)	C10-C11	1.440(2)
O1-C2	1.273(2)	C11-C15	1.400(2)
O2-C2	1.240(2)	C11-C12	1.405(2)
O3-C3	1.428(2)	C12-C13	1.375(3)
O3-C4	1.421(2)	C13-C14	1.397(3)
N1-C1	1.485(2)	C15-C16	1.435(2)
N1-C4	1.479(3)	N2-C5	1.333(2)
N2-C16	1.357(2)	N3-C14	1.326(2)
N3-C15	1.357(2)	C1-C3	1.545(3)
C1-C2	1.532(2)	C5-C6	1.405(3)
O5-N4	1.246(2)	C6-C7	1.369(3)
O6-N4	1.235(2)	O7-N4	1.254(2)

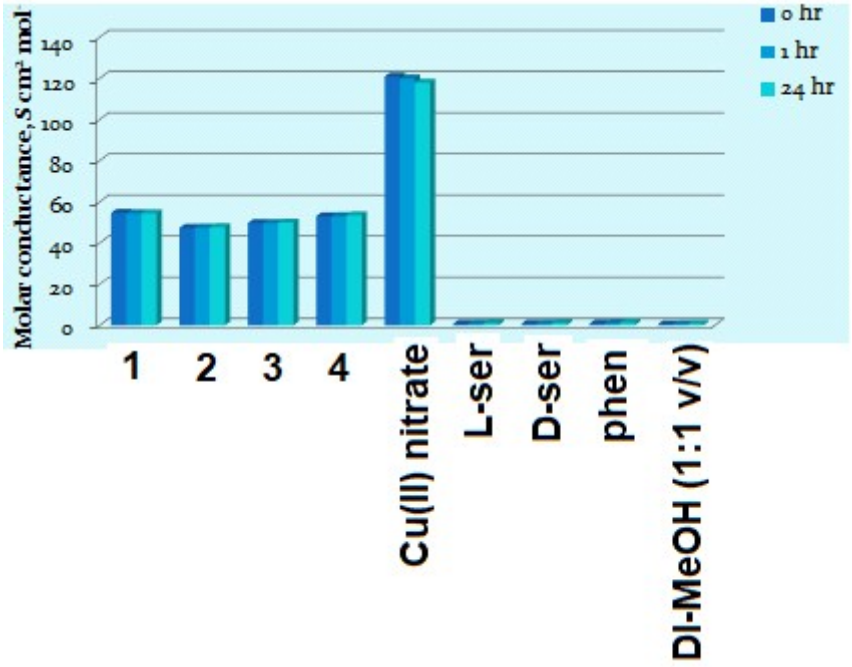
Bond Angles (Degrees)			
O1-Cu1-O4	92.33(6)	C1-N1-H1N	107.7(14)
O1-Cu1-N1	84.86(6)	Cu1-N1-H1N	110.5(13)
O1-Cu1-N2	174.05(6)	O2-C2-C1	117.96(16)
O1-Cu1-N3	92.31(5)	O1-C2-C1	116.63(15)
O4-Cu1-N1	86.70(7)	O1-C2-O2	125.40(16)
O4-Cu1-N2	87.04(7)	O3-C3 -C1	105.50(14)
O4-Cu1-N3	105.12(7)	O3-C4-N1	104.96(17)
N1-Cu1-N2	101.01(6)	N2-C5-C6	121.95(17)

N1-Cu1-N3	167.97(8)	C5-C6-C7	120.00(16)
N2-Cu1-N3	82.16(5)	C6-C7-C8	119.62(17)
Cu1-O1-C2	115.14(12)	C7-C8-C16	116.43(15)
C3-O3-C4	105.75(14)	C7-C8-C9	124.98(16)
Cu1-N1-C1	106.83(11)	C9-C8-C16	118.59(15)
Cu1-N1-C4	117.65(12)	C8-C9-C10	121.77(16)
C1-N1-C4	103.03(14)	C9-C10-C11	120.79(16)
Cu1-N2-C5	129.86(12)	C12-C11-C15	117.43(16)
Cu1-N2-C16	111.44(10)	C10-C11-C12	124.23(16)
C5-N2-C16	118.04(15)	C10-C11-C15	118.34(16)
Cu1-N3-C14	128.57(12)	C11-C12-C13	118.99(17)
Cu1-N3-C15	113.29(11)	C12-C13-C14	119.74(16)
C14-N3-C15	118.14(15)	N3-C14-C13	122.47(17)
N3-C15-C16	115.92(15)		
Cu1-O4-H2O	120.0(15)	N3-C15-C11	123.18(16)
Cu1-O4-H1O	124.7(19)	C11-C15-C16	120.90(15)
C2-C1-C3	112.53(15)	C8-C16-C15	119.54(15)
N1-C1-C3	104.52(15)	N2-C16-C8	123.96(14)
N1-C1-C2	110.78(14)	N2-C16-C15	116.50(14)
O6-N4-O7	119.00(16)	O5-N4-O6	120.23(17)
O5-N4-O7	120.77(16)		

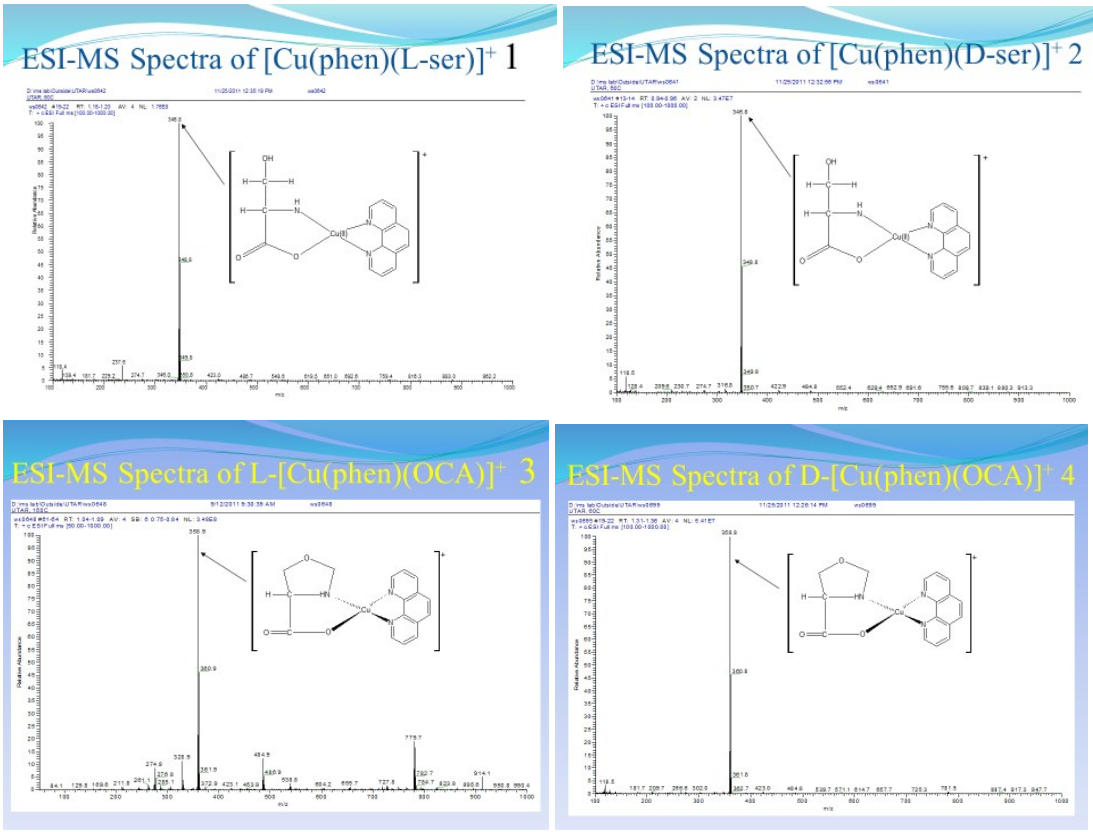
3. ESI Table S3 (UV-Visible Absorption)

Complex	λ_{max} (nm), ε($mol^{-1}dm^3$ cm^{-1})	Assignment
L-[Cu(phen)(L-ser)(H_2O)]NO_3 **(1)**	224 (34 007)	π→π*
	273 (32 862)	π→π*
	613 (62)	d-d
D-[Cu(phen)(D-ser)(H_2O)]NO_3 **(2)**	224 (35 173)	π→π*
	273 (33 960)	π→π*
	613 (62)	d-d
L-[Cu(phen)(OCA)(H_2O)]NO_3 **(3)**	224 (33 423)	π→π*
	273 (32 147)	π→π*
	623 (62)	d-d
D-[Cu(phen)(OCA)(H_2O)]NO_3 **(4)**	225 (65 870)	π→π*
	273 (62 897)	π→π*
	622 (62)	d-d

4. ESI Figure S1



5. ESI Fig. S2.1–S2.4 (Electrospray Ionization-Mass spectra)



6. ESI Fig. S3 (Fluorescence emission)