Electronic supplementary information

DNA binding, molecular docking and apoptotic inducing activity of nickel(II), copper(II) and zinc(II) complexes of pyridine-based tetrazolo[1,5-*a*]pyrimidine ligands

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Table S1 Crystal data and structure refinement for ligands **L[1&2]** and complex **6**.

	L[1]	**L[2]**	**6**
Empirical Formula	$C_{13}H_{14}N_6O_2$	$C_{13}H_{16}N_6O_3$	$C_{28}H_{37}N_{12}O_{6.5}Cl_2Zn$
Formula Weight	286.30	304.32	781.97
Temperature (K)	293(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Orthorhombic	Monoclinic
Space group	P-1	Pbca	C2/c
Unit cell dimensions			
a (Å)	8.282(5)	9.3144(3)	10.4600(4)
b (Å)	9.501(5)	17.8682(5)	13.5070(5)
c (Å)	9.604(5)	18.0638(6)	26.6520(9)
α (°)	106.753(5)	90	90
β (°)	100.835(5)	90	93.851(2)
γ (°)	100.556(5)	90	90
Volume ($Å^3$)	687.7(7)	3006.39(16)	3757.0(2)
Z	2	8	4
Calculated density (Mg/m^{-3})	1.383	1.345	1.382
Adsorption coefficient (mm^{-1})	0.099	0.100	0.853
F(000)	300	1280	1620
Crystal size (mm^3)	0.30 x 0.20 x 0.20	0.30 x 0.25 x 0.15	0.30 x 0.20 x 0.20
Index ranges	$-9 \le h \le 9$,	$-11 \le h \le 11$,	$-11 \le h \le 11$,
	$-11 \le k \le 11$,	$-21 \le k \le 21$,	$-14 \le k \le 14$,
	$-11 \le l \le 11$	$-21 \le l \le 20$	$-29 \le l \le 29$
Reflections collected	8477	16734	11512
Independent reflections	2420[R(int) = 0.0217]	2640 [R(int) = 0.0459]	2751 [R(int) = 0.1363]
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	2420/0/199	2640/19/232	2751/61/281
GOF on F^2	1.066	1.054	0.971
Final R indices [$I<2\sigma(I)$]	R1 = 0.0399, *w*R2 = 0.1091	R1 = 0.0468, *w*R2 = 0.1142	R1 = 0.0621, *w*R2 = 0.1518
R indexes (all data)	R1 = 0.0444, *w*R2 = 0.1141	R1 = 0.0739, *w*R2 = 0.1298	R1 = 0.1965, *w*R2 = 0.1873
Largest diff. peak and hole (e. $Å^{-3}$)	0.260 and −0.222	0.185 and −0.205	0.468 and −0.306

Table S2. Selected bond lengths (Å) and bond angles (º) for ligand **L**[1].

Bond lengths (Å)			
C(1)-N(1)	1.324(2)	C(3)-C(11)	1.470(2)
C(1)-N(5)	1.352(2)	C(4)-C(5)	1.494(2)
C(2)-N(1)	1.4630(19)	N(1)-N(2)	1.3562(19)
C(2)-C(6)	1.522(2)	N(2)-N(3)	1.288(2)
C(2)-C(3)	1.523(2)	N(3)-N(4)	1.367(2)
C(3)-C(4)	1.354(2)		

Bond angles (º)			
N(4)-C(1)-N(5)	129.42(14)	C(6)-N(6)-C(7)	117.17(14)
N(1)-C(1)-N(5)	120.83(13)	C(1)-N(1)-N(2)	108.28(12)
N(1)-C(2)-C(6)	108.36(12)	C(1)-N(1)-C(2)	125.56(13)
C(6)-C(2)-C(3)	113.49(12)	N(3)-N(2)-N(1)	105.94(13)
C(6)-C(2)-H(2)	109.1(9)	N(2)-N(3)-N(4)	111.37(13)
C(8)-C(9)-C(10)	119.15(15)	C(1)-N(4)-N(3)	104.72(13)
N(6)-C(7)-H(7)	118.3	C(1)-N(5)-C(4)	119.50(13)

Table S3. Selected interatomic distance (Å) and angles (°) for ligand **L**[1].

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (°)
N(5)-H(5D)...N(4)#1	0.87(2)	2.05(2)	2.906(2)	165.3(18)

Symmetry transformations used to generate equivalent atoms: #1 –x, –y, –z+1

Table S4. Selected bond lengths (Å) and bond angles (°) for ligand **L²**.

. **Bond lengths (Å)**			
C(3)-C(4)	1.457(3)	C(6)-N(1)	1.348(3)
C(4)-C(5)	1.355(3)	C(7)-N(5)	1.463(3)
C(4)-C(7)	1.526(3)	C(7)-C(8)	1.522(3)
C(5)-N(1)	1.377(3)	N(2)-N(3)	1.366(3)
C(5)-C(13)	1.502(3)	N(3)-N(4)	1.291(3)
C(6)-N(2)	1.318(3)	N(4)-N(5)	1.360(2)
C(6)-N(5)	1.323(3)		
Bond angles (°)			
N(2)-C(6)-N(5)	109.7(2)	C(6)-N(1)-C(5)	119.82(19)
N(2)-C(6)-N(1)	129.5(2)	C(6)-N(2)-N(3)	104.66(19)
N(5)-C(6)-N(1)	120.8(2)	N(4)-N(3)-N(2)	111.62(18)
N(5)-C(7)-C(8)	108.96(15)	N(3)-N(4)-N(5)	105.54(18)
N(5)-C(7)-C(4)	106.88(16)	C(6)-N(5)-N(4)	108.44(17)
C(8)-C(7)-C(4)	114.29(16)	C(6)-N(5)-C(7)	127.55(18)
N(5)-C(7)-H(7)	108.9	N(4)-N(5)-C(7)	123.86(16)

Table S5. Selected interatomic distance (Å) and angles (°) for ligand **L¹**.

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (°)
N(1)-H(1)...N(6)#1	0.917 (16)	1.892(17)	2.805(3)	173(2)
O(1W)-H(1W)...N(2)#2	0.964(18)	2.077(19)	3.040(3)	176(4)
O(1W)-H(2W)...O(2)#3	0.961(19)	2.01(2)	2.931(3)	160(4)

Symmetry transformations used to generate equivalent atoms: #1 –x+3/2,y–1/2,z ; #2 –x+2, –y, –z+1; #3 x+1/2,y, –z+3/2

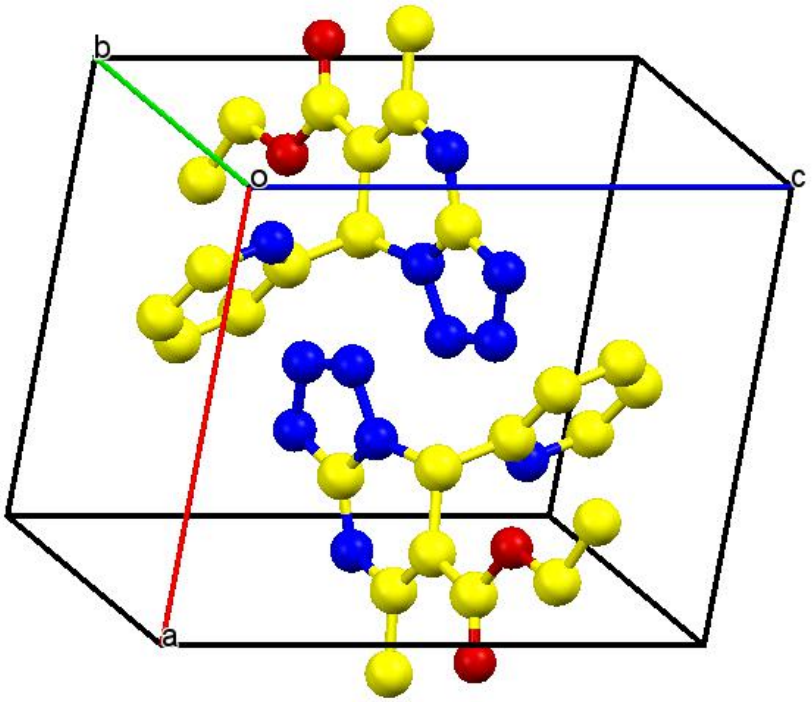


Fig. S1. Crystal packing diagram of ligand L^1 projecting along the crystallographic *b*-axis.

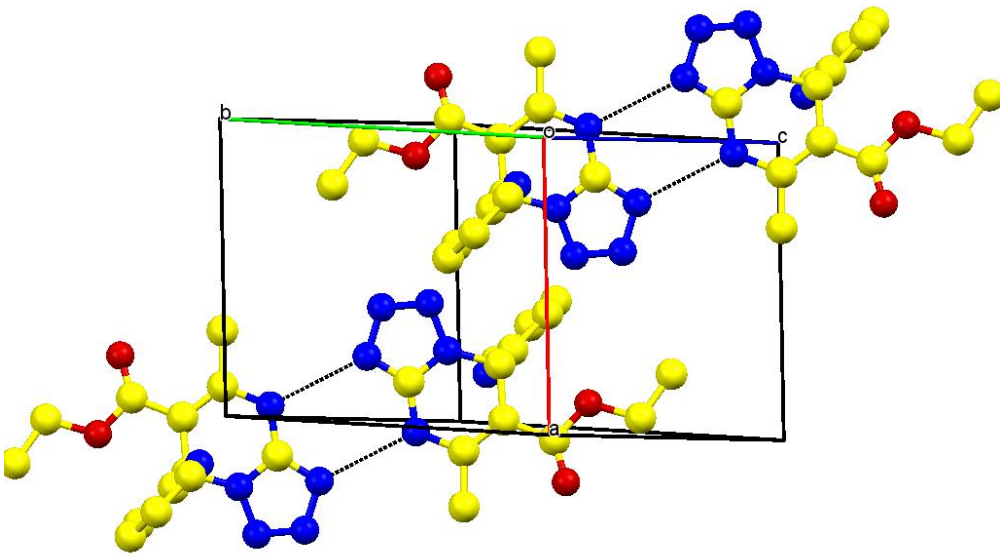


Fig. S2. View of crystal lattice packing showing the internuclear hydrogen bonding of ligand L^1.

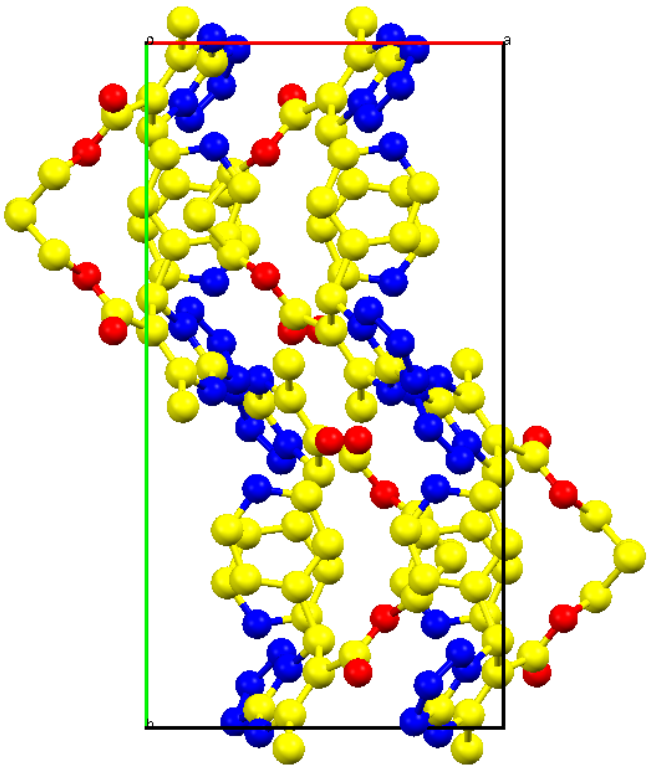


Fig. S3. Crystal packing diagram of ligand L^2 projecting along the crystallographic *c*-axis.

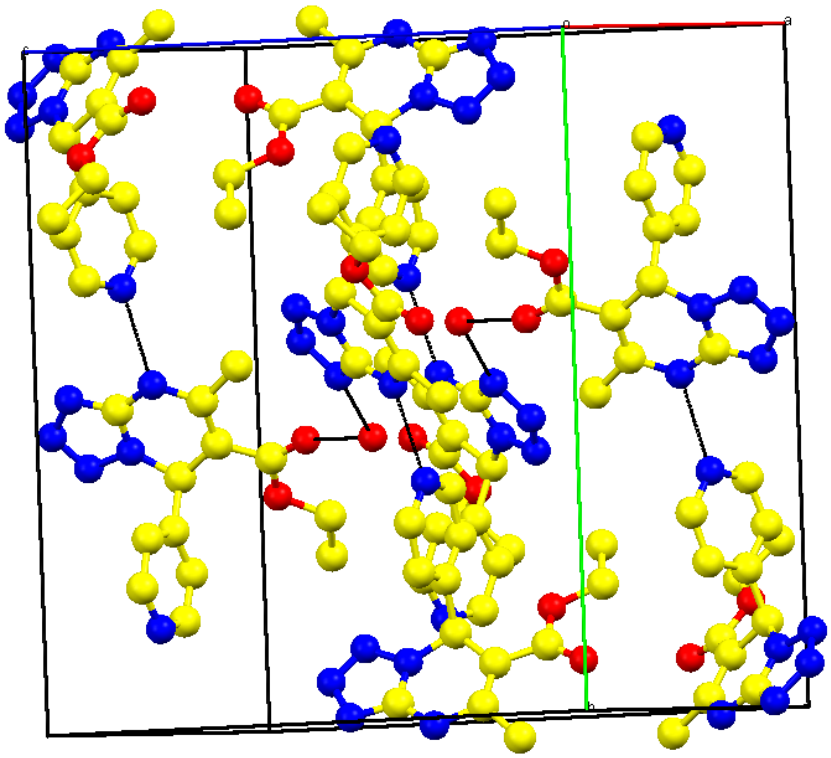


Fig. S4. View of crystal lattice packing showing the internuclear hydrogen bonding of ligand L^2.

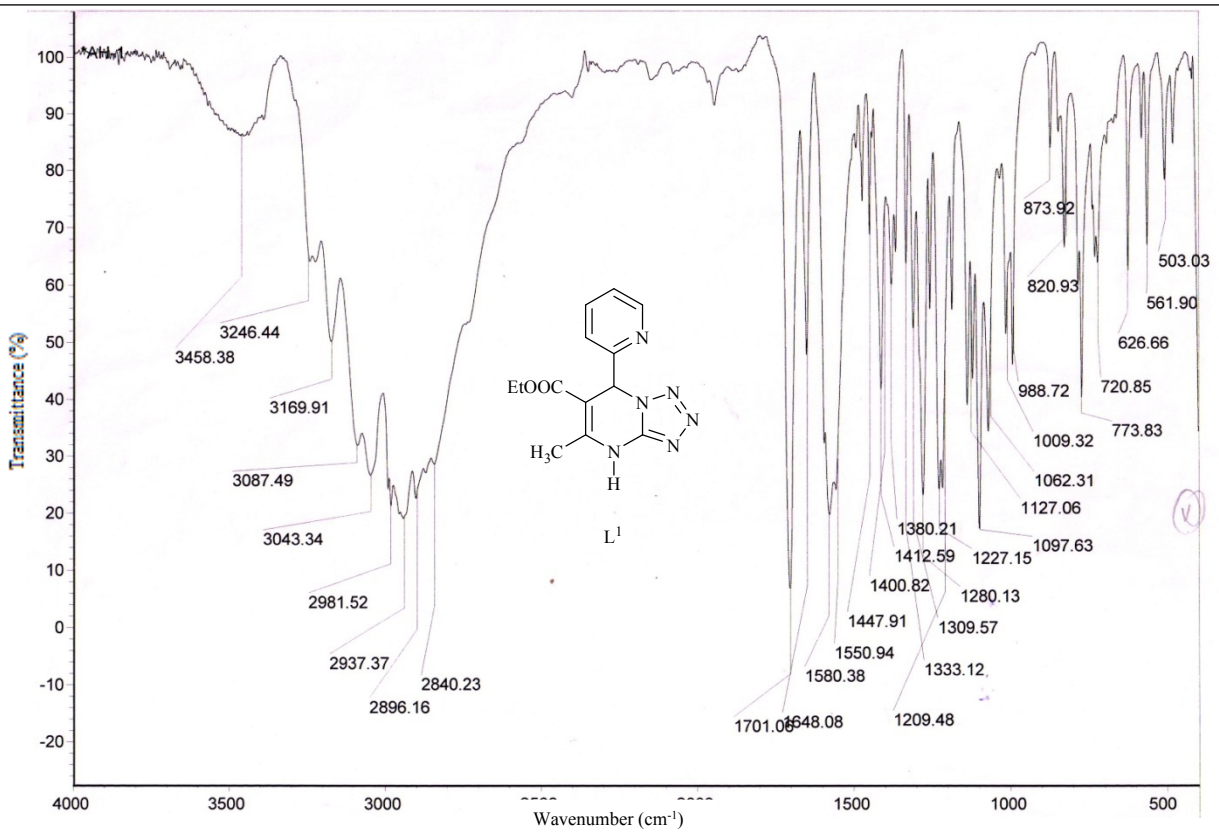


Fig. S5. FT IR spectrum of ligand L^1

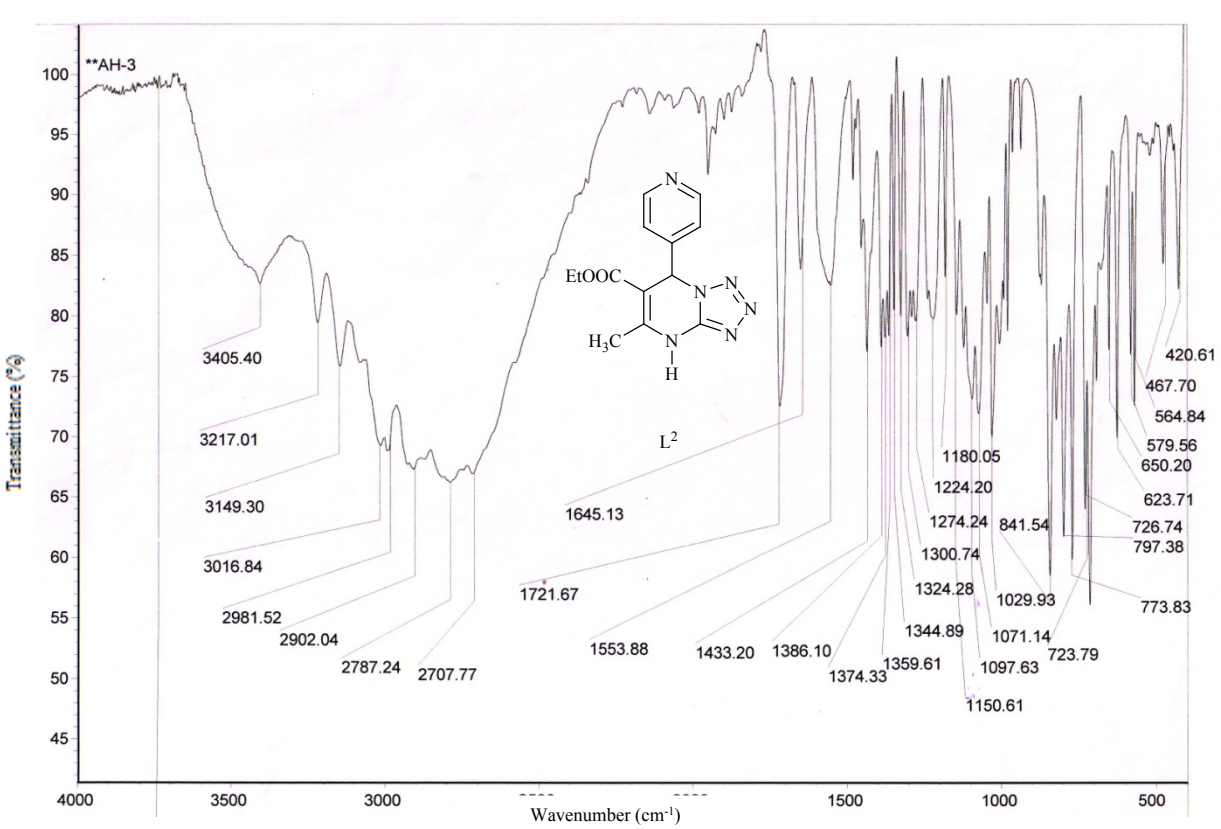


Fig. S6. FT IR spectrum of ligand L^2

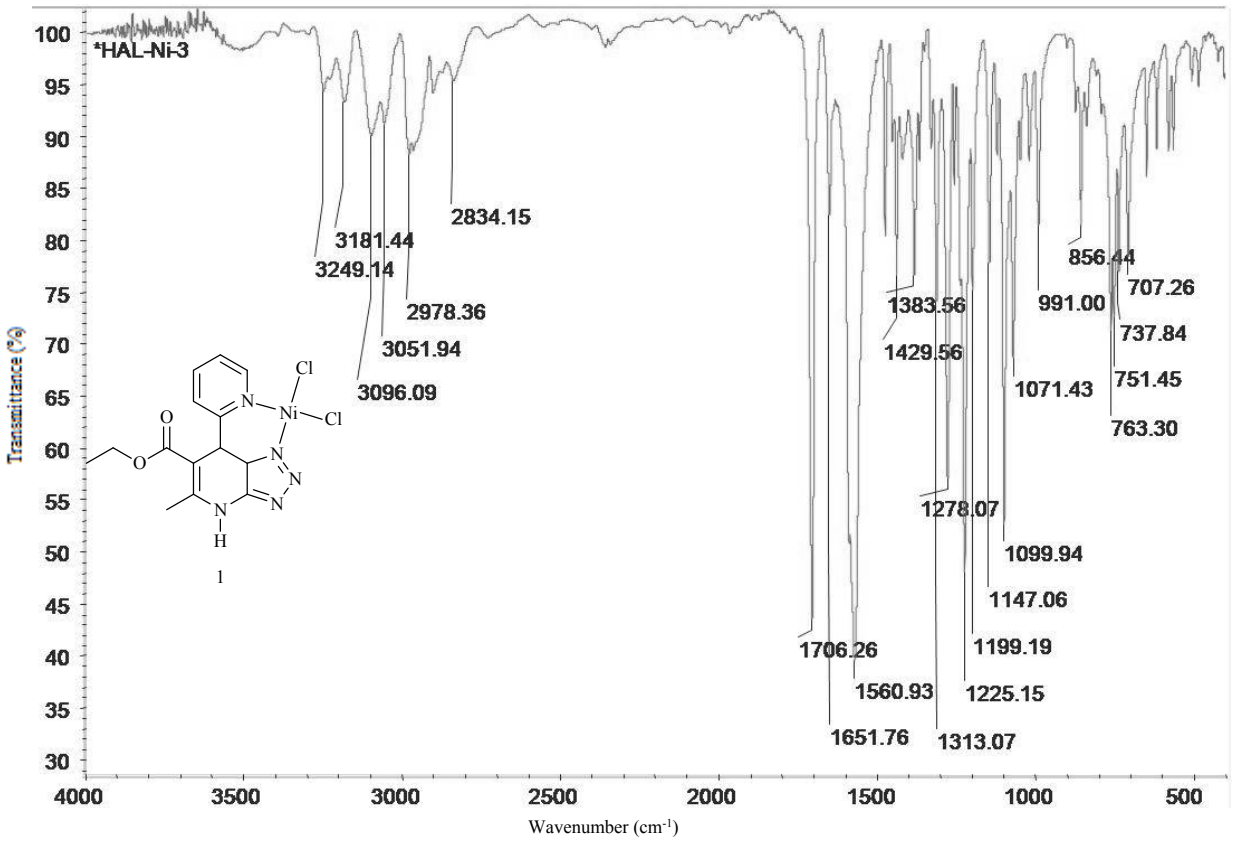


Fig. S7. FT IR spectrum of Complex 1

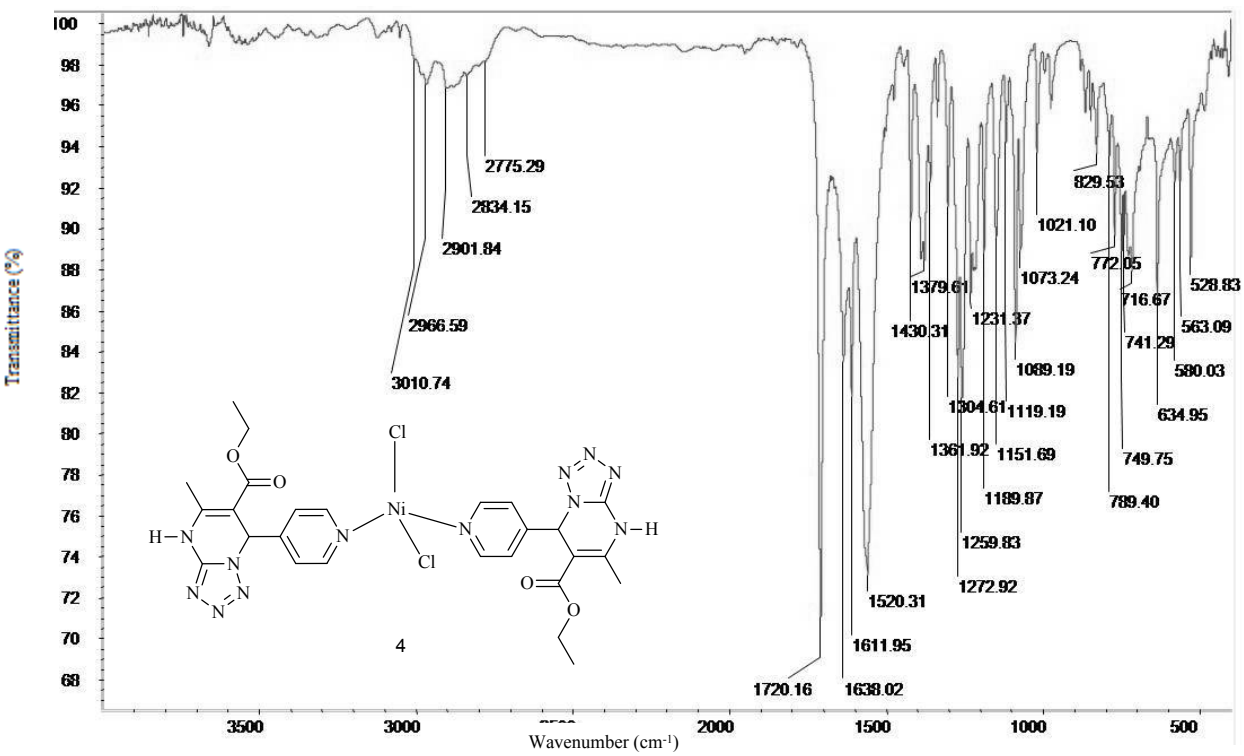


Fig. S8. FT IR spectrum of complex 4

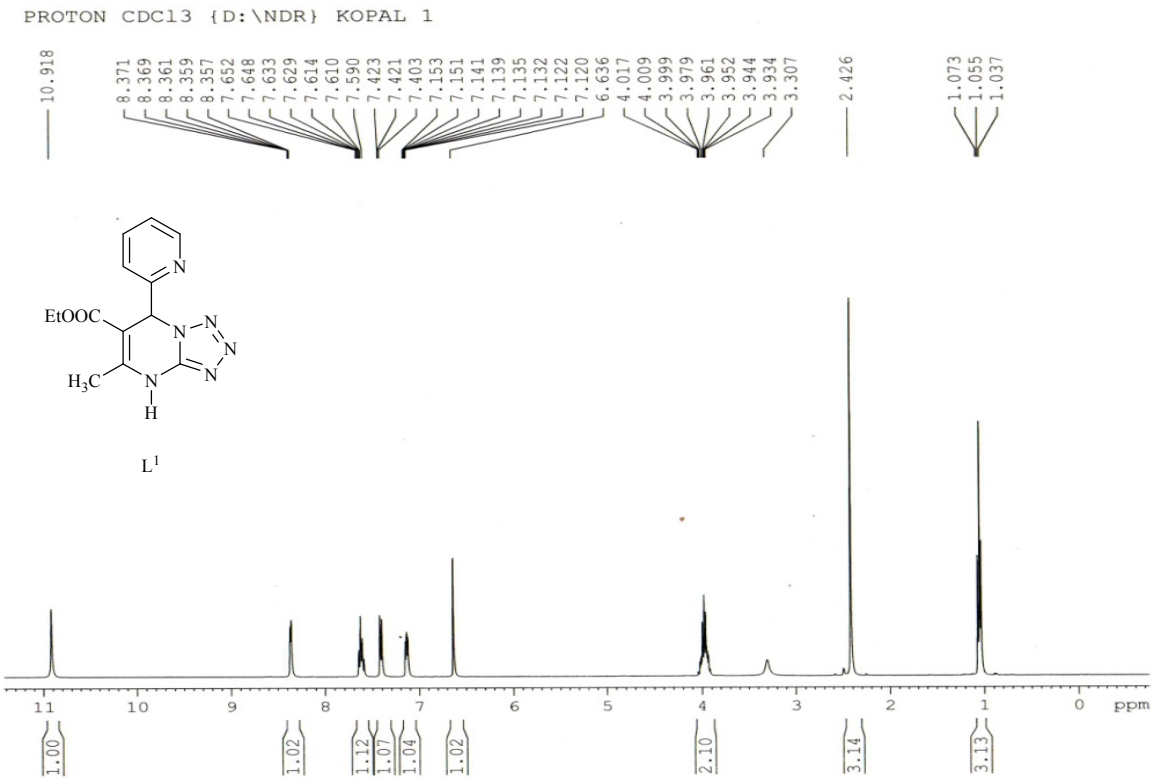


Fig. S9. ^{1}H NMR spectrum of ligand L^{1}

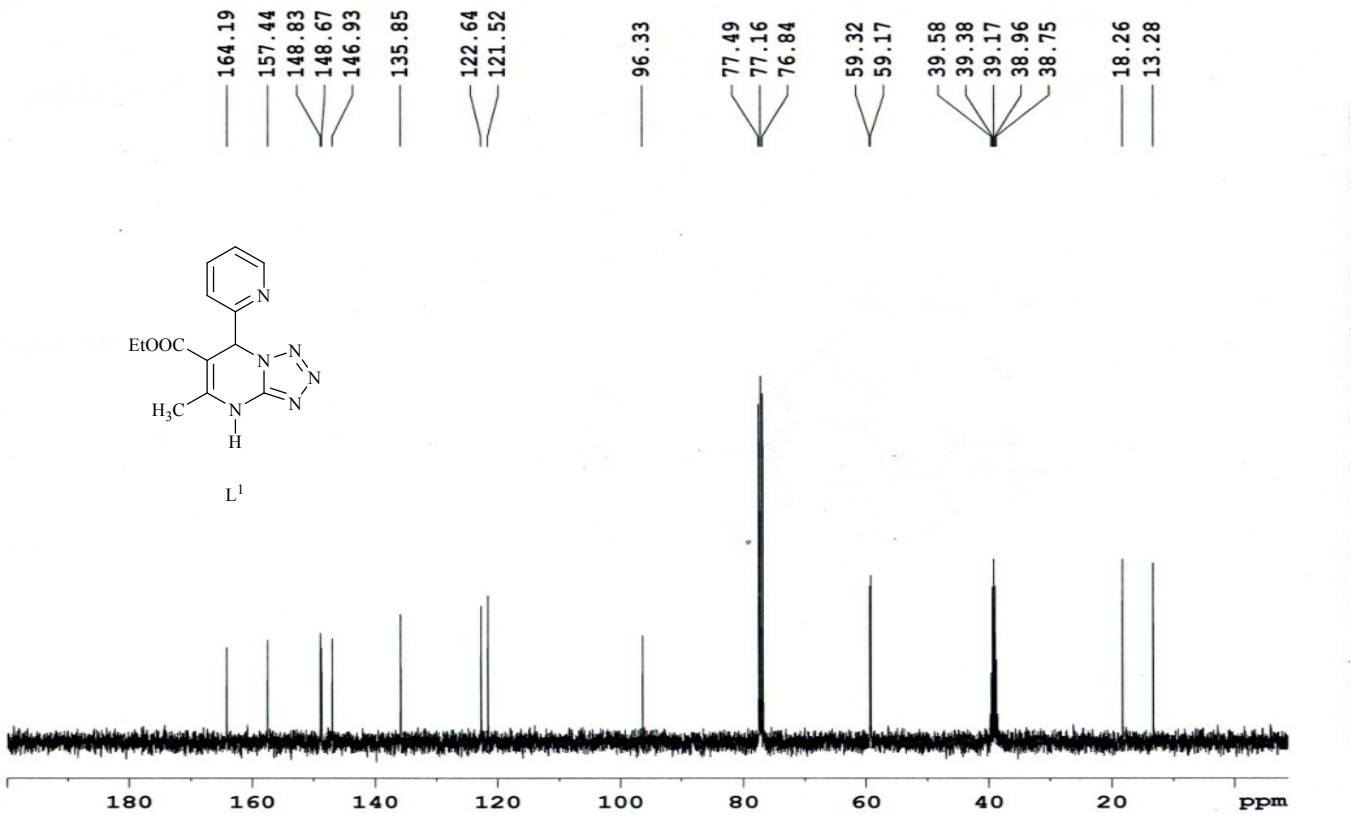
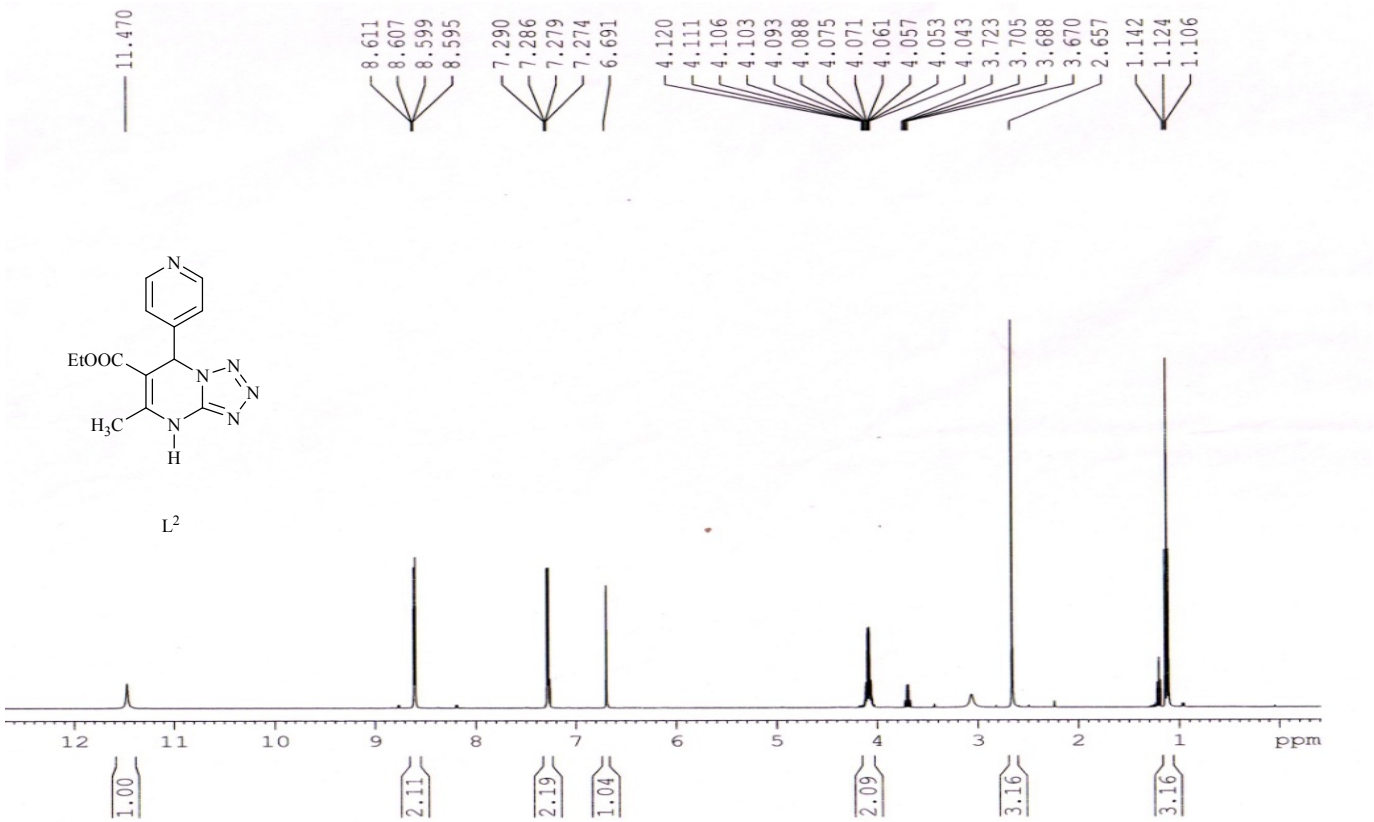
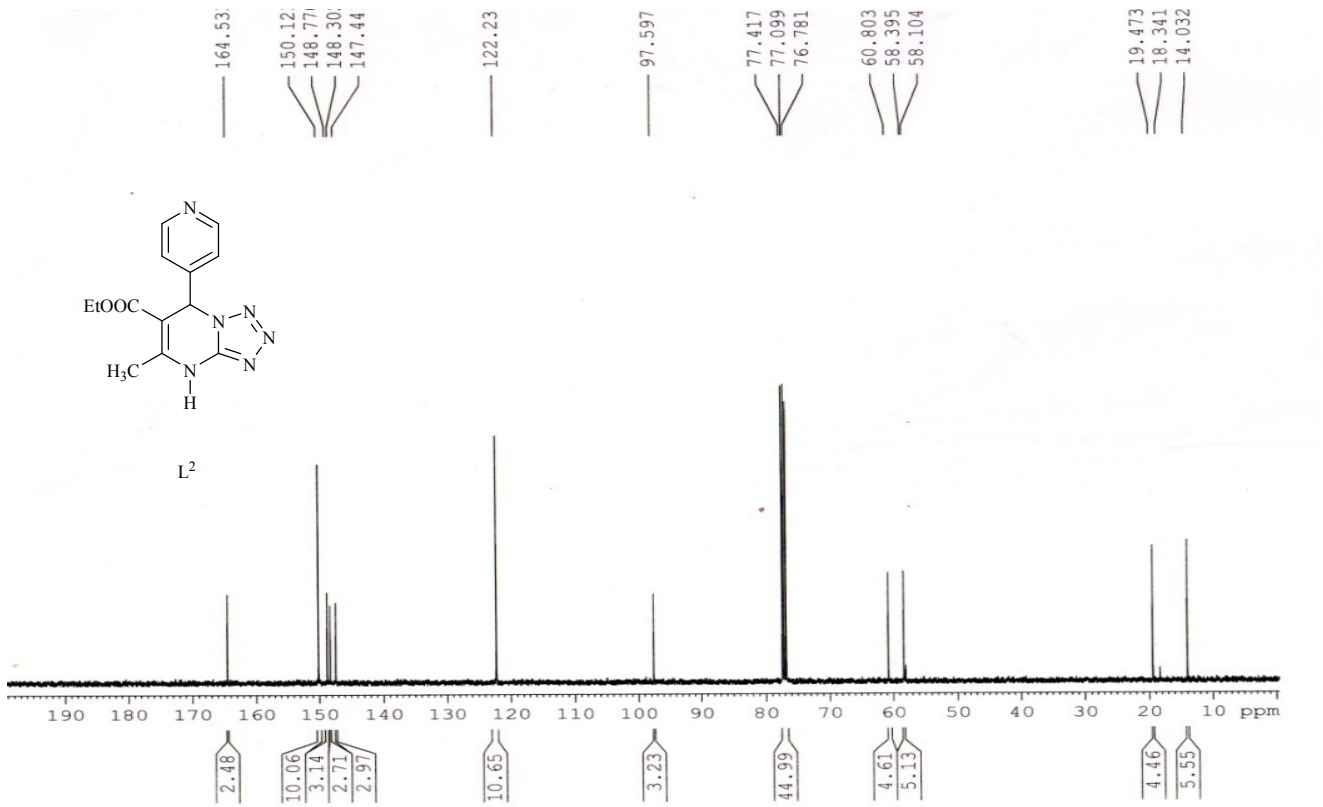


Fig. S10. ^{13}C NMR spectrum of ligand L^{1}



L^2

Fig. S11. ^{1}H NMR spectrum of ligand L^2



L^2

Fig. S12. ^{13}C NMR spectrum of ligand L^2

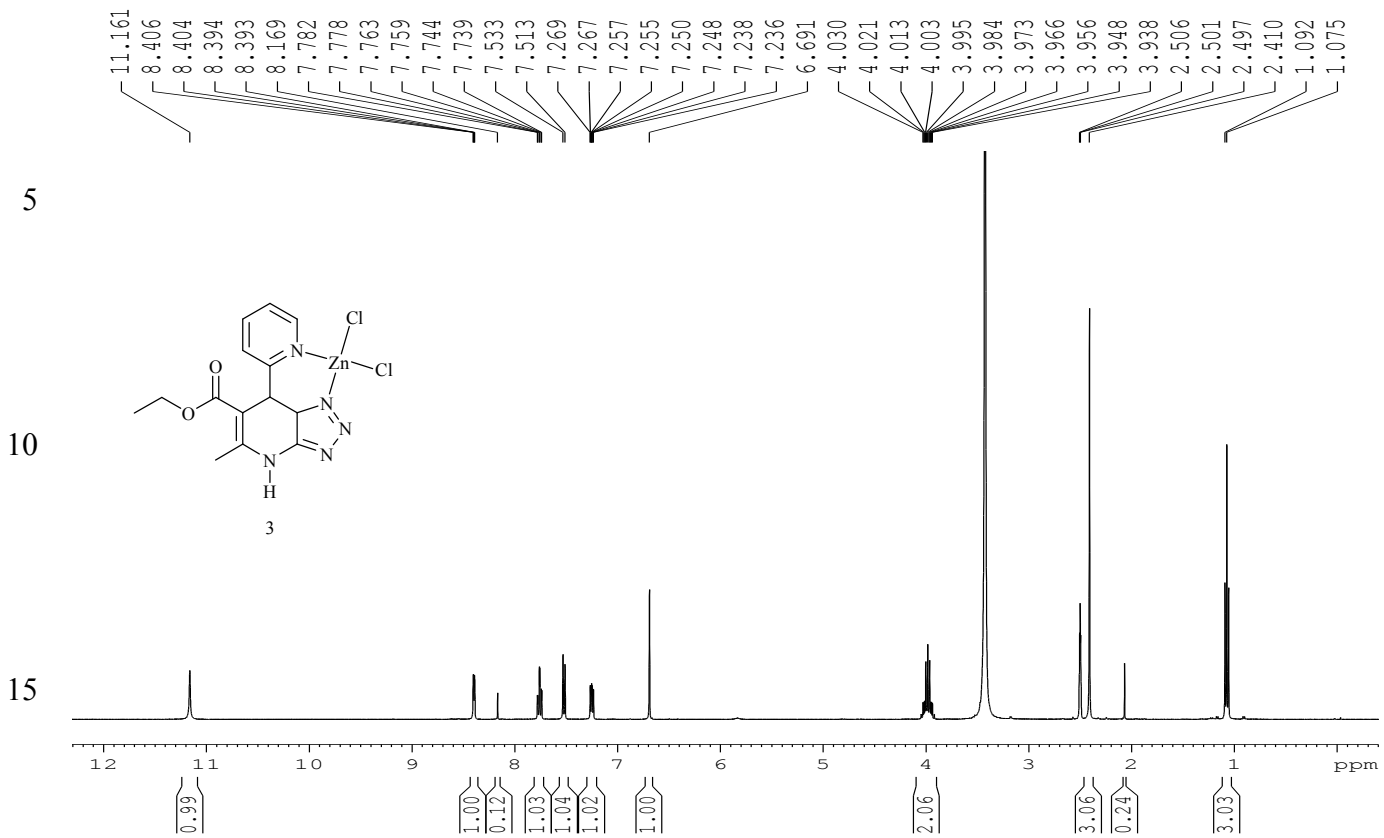


Fig. S13. ^{1}H NMR spectrum of complex 3

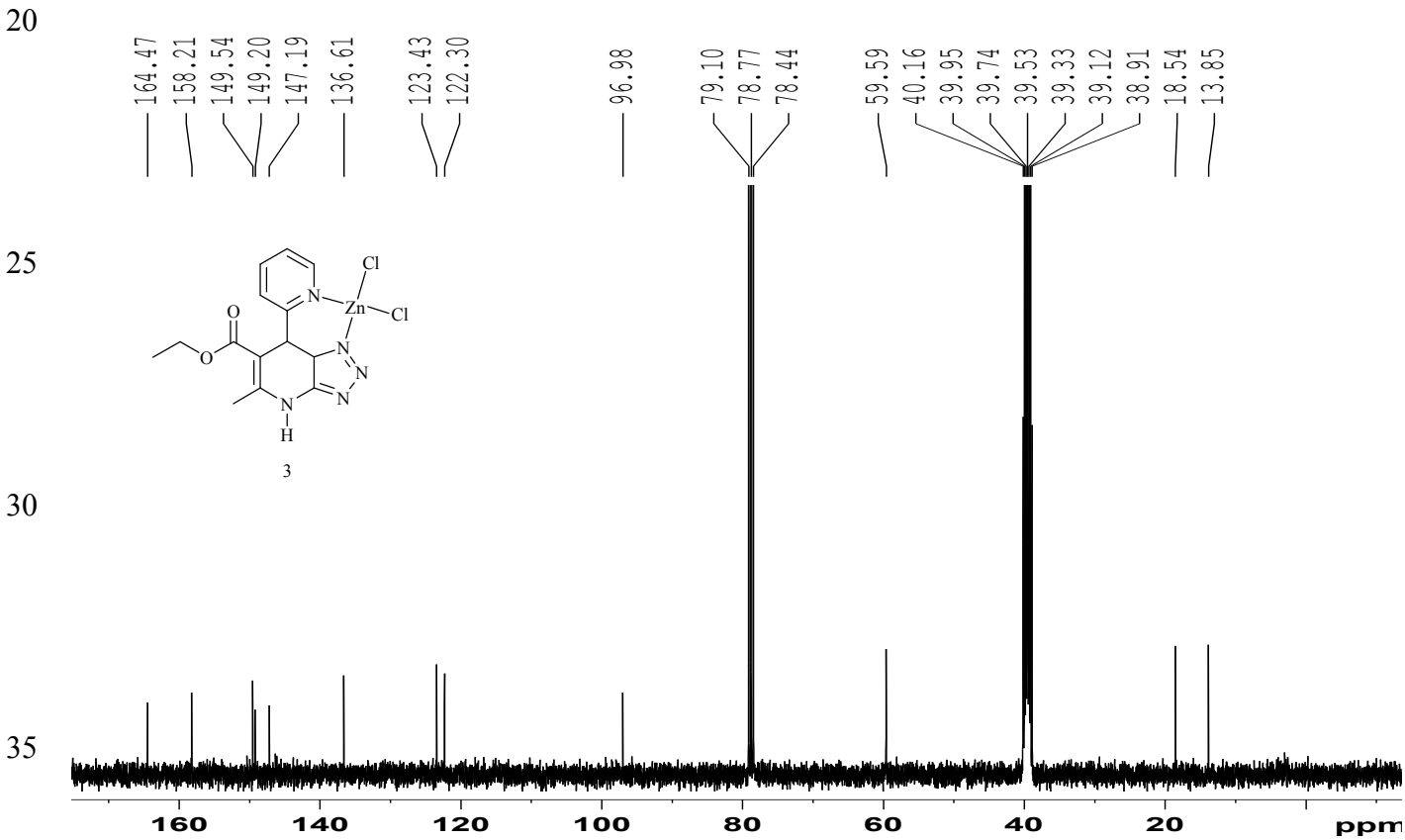


Fig. S14. ^{13}C NMR spectrum of complex 3

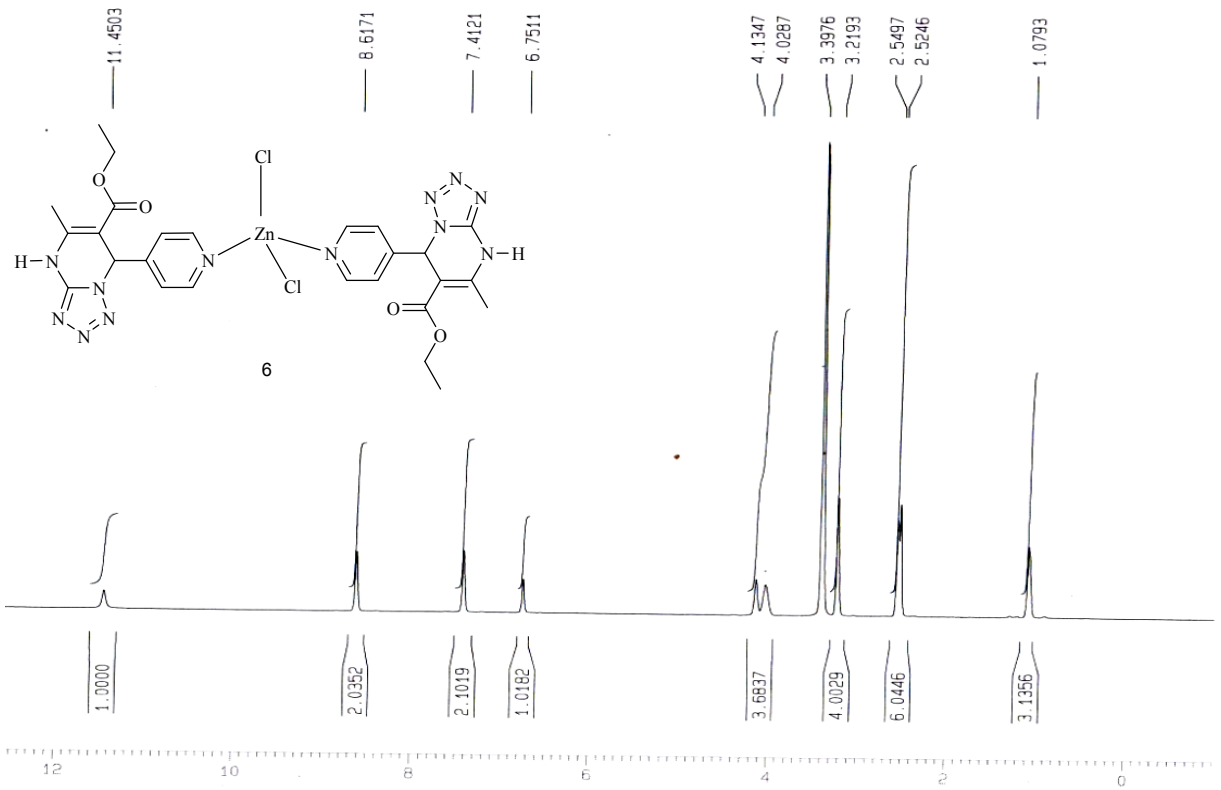


Fig. S15. ^{1}H NMR spectrum of complex 6

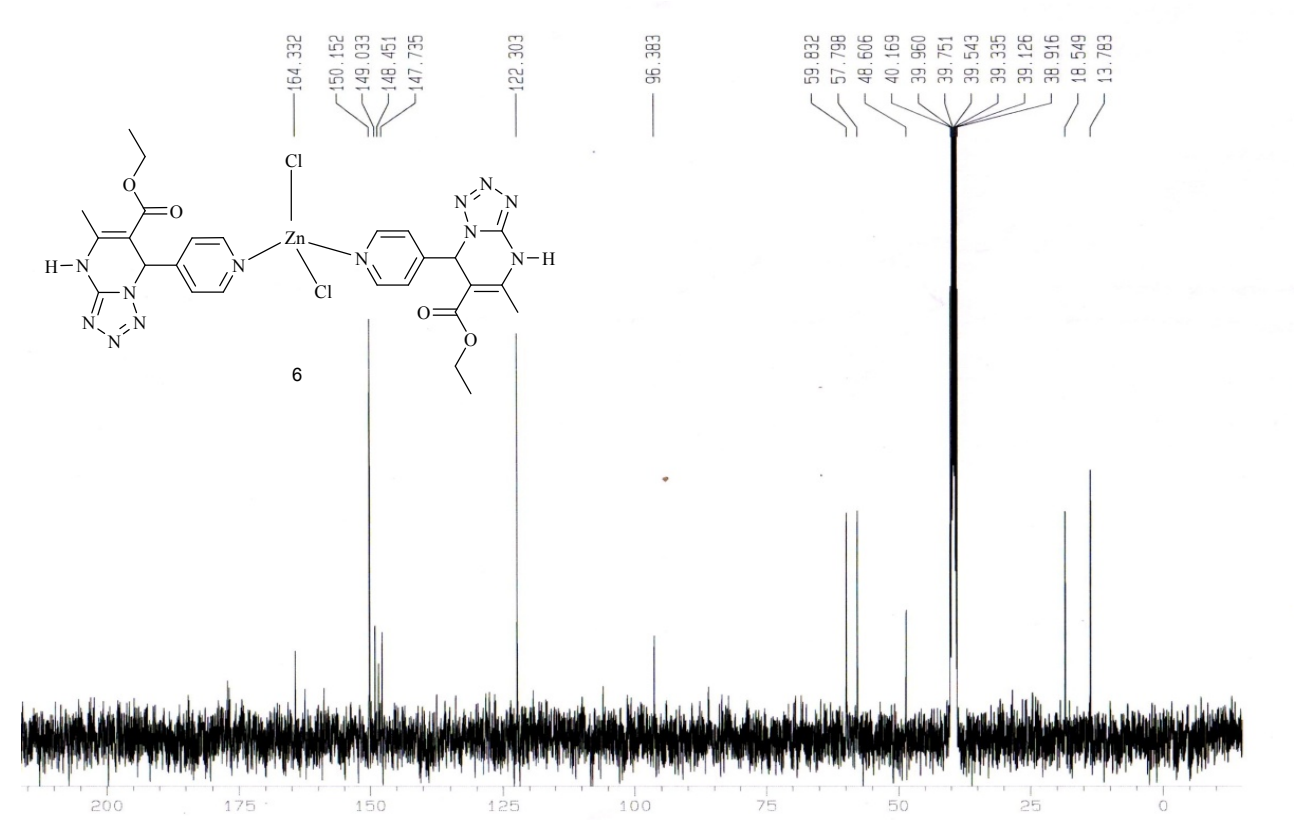


Fig. S16. ^{13}C NMR spectrum of complex 6

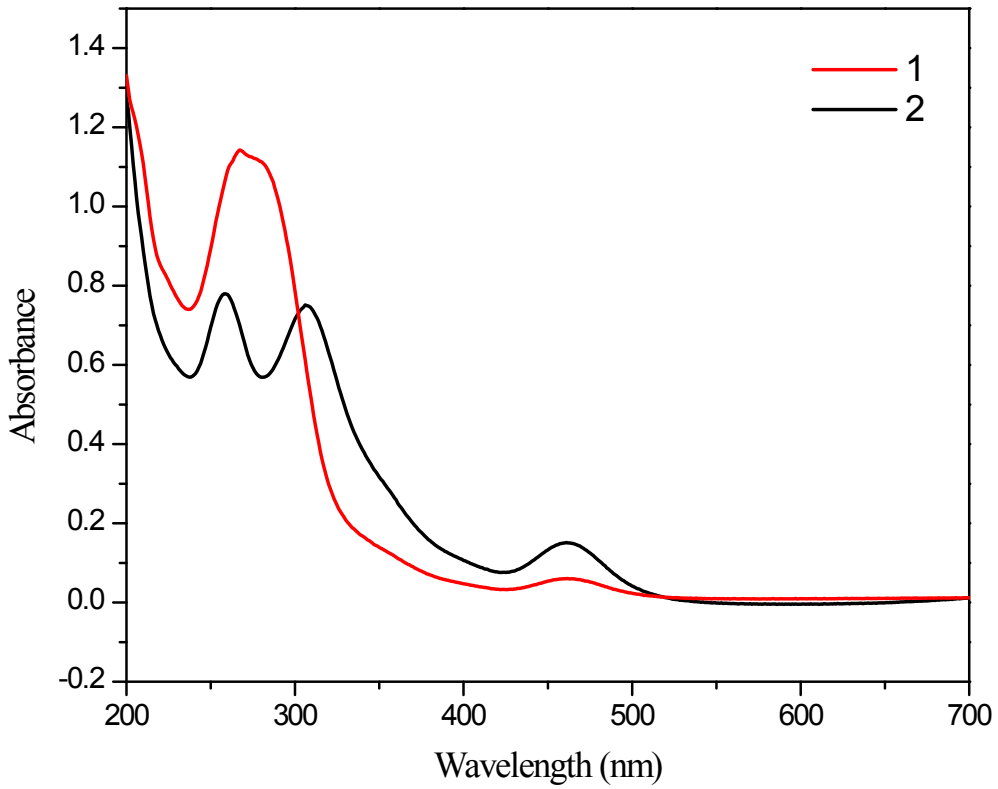


Fig. S17. UV-Vis spectra of complexes 1 & 2

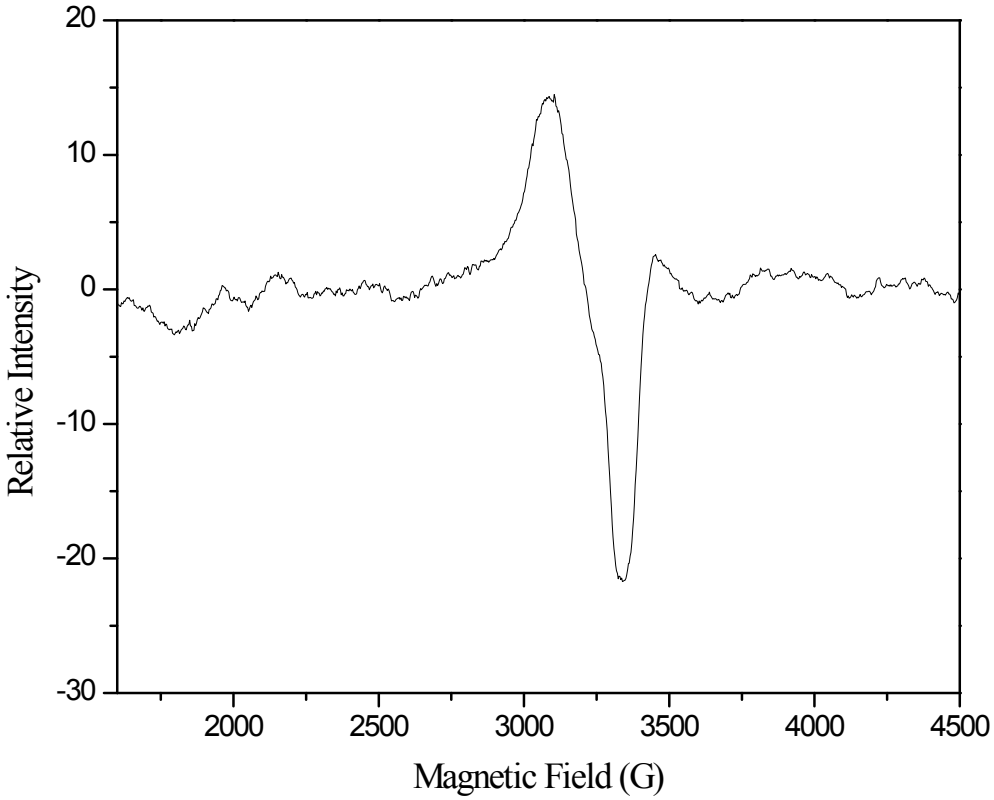


Fig. S18. X- band EPR spectrum of complex 2