Supplementary Material

Experimental Section

1 Molecular docking

The molecular docking studies were carried out using the AutoDock Tools (ADT) version 1.5.6 and AutodockVinaprogrammes[1,2].The crystal structures of human human topoisomerase I (PDB ID: 1T8i).In topoisomerase I, the indinoisoquinoline ligand was removed from the crystallographic coordinate set.

References

[1] G.M. Morris, R. Huey, W. Lindstrom, M.F. Sanner, R.K. Belew, D.S. Goodsell, A.J. Olson, J. Comput. Chem. 30 (2009) 2785–2791.

[2] O.Trott, A. J. Olson, J. Comput. Chem. 31 (2010) 455–461.

Table S1 Selected bond lengths [Å] and angles [°] in complexes **C1-C5**.

C1				**C2**			
Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Zn1	2156.0(4)	7547.2(4)	7757.4(2)	Zn1	3778.5(4)	6547.2(4)	7307.8(2)
Zn2	3453.2(4)	4048.1(4)	6885.3(2)	Zn2	9716.4(6)	5000	5000
S1	1227.6(11)	7924.0(13)	9102.0(6)	Zn3	7093.1(6)	5000	5000
S2	1749.3(9)	9887.6(10)	6999.7(6)	S1	3198.4(12)	6115.9(10)	6570.8(6)
S3	1927.8(9)	4026.4(9)	5868.5(5)	S2	2755.1(10)	7460.8(9)	7632.5(7)
S4	5548.4(10)	1928.1(10)	7374.0(7)	S3	6305.2(10)	3924.7(8)	5311.4(5)
N1	3661(3)	5124(3)	8382.0(15)	S4	10706.7(11)	5029.4(10)	5663.5(6)
N2	40(3)	7871(3)	7480.8(17)	N1	4459(3)	6288(3)	8039.9(16)
N3	-972(3)	8209(3)	8061.6(18)	N2	3856(3)	5263(2)	7395.7(15)
N4	-1519(4)	8669(4)	9356(2)	N3	3700(3)	4734(3)	7037.5(16)
N5	4318(3)	7215(3)	7795.7(17)	N4	3312(5)	4599(4)	6292(2)
N6	4678(3)	8229(3)	7380(2)	N5	4427(3)	7616(2)	7088.6(15)
N7	3936(4)	10343(4)	6521(3)	N6	4080(3)	8366(3)	7224.3(16)
N8	2052(3)	7001(3)	6350.8(16)	N7	3038(4)	9064(3)	7623(2)
N9	1780(3)	4328(3)	7647.5(15)	N8	8628(3)	5579(2)	4506.5(16)
N10	515(3)	4409(3)	7323.1(17)	N9	9638(3)	6273(3)	5167.5(16)
N11	-659(3)	4310(3)	6208.7(19)	N10	10069(3)	6609(3)	5539.0(16)
N12	4912(3)	4837(3)	6574.3(16)	N11	10986(4)	6369(3)	6142.2(19)
N13	6356(3)	4021(3)	6863.8(17)	N12	7583(3)	4182(3)	4541.7(15)
N14	8069(3)	1867(4)	7572(2)	N13	7360(3)	3347(3)	4586.6(15)
O1	5339(5)	9432(5)	8853(3)	N14	6515(3)	2431(3)	4988(2)

C3				**C4**			
Atom	***x***	***y***	***z***	**Atom**	***x***	***y***	***z***
Zn1	503.9(4)	1964.52(17)	7854.0(4)	Zn1	2870.1(3)	4651.6(8)	5012.6(3)
Zn2	3278.3(4)	1899.89(18)	7605.4(4)	S1	1927.7(6)	6640(2)	5364.5(8)
S1	50.1(12)	2268.9(4)	9224.7(10)	S2	2526.7(6)	2381.1(19)	5856.0(8)
S2	-907.0(11)	1579.8(5)	6797.7(10)	N1	3316.0(19)	4045(5)	4048(2)
S3	3709.7(12)	2213.6(4)	6256.4(10)	N2	2094.0(19)	5251(5)	3865(2)
S4	4497.2(11)	1421.3(5)	8652.4(10)	N3	1441.0(19)	5742(5)	3832(2)
N1	1250(3)	2038.3(13)	6480(2)	N4	644(2)	6690(6)	4410(3)
N2	567(3)	2678.3(12)	7538(2)	N5	3747(2)	2356(6)	5348(2)
N3	344(3)	3017.0(12)	8140(3)	N6	3851(2)	1610(6)	6091(2)
N4	-235(4)	3158.0(13)	9468(3)	N7	3396(2)	604(6)	7052(3)
N5	931(3)	1276.1(13)	8303(2)	Cl1	3693.7(6)	6637.5(19)	5693.0(8)
N6	326(3)	904.6(14)	7882(3)	**C5**			
N7	-1179(4)	684.8(17)	6793(4)	Zn1	5835.33(14)	1189.07(19)	1946.20(18)
N8	2398(3)	1954.5(13)	8976(3)	S1	6024.7(4)	2098.5(5)	777.2(4)
N9	3227(3)	2589.6(13)	7975(2)	S2	6789.0(3)	538.5(5)	2531.7(5)
N10	3453(3)	2941.9(13)	7405(3)	N1	4664.2(10)	1063.7(14)	1526.3(12)
N11	3964(4)	3105.7(13)	6035(3)	N2	5782.5(9)	2546.0(14)	2490.8(13)
N12	2577(3)	1273.6(13)	7074(3)	N3	5859(1)	3364.5(16)	2028.8(14)
N13	3043(3)	857.5(13)	7434(3)	N4	6108.4(15)	4015.0(18)	814.6(18)
N14	4460(4)	511.7(15)	8474(3)	N5	5606.3(9)	-256.6(14)	1776.6(11)
				N6	6025.9(11)	-966.6(15)	2024.4(13)
				N7	6975.3(11)	-1361.2(17)	2619.1(17)

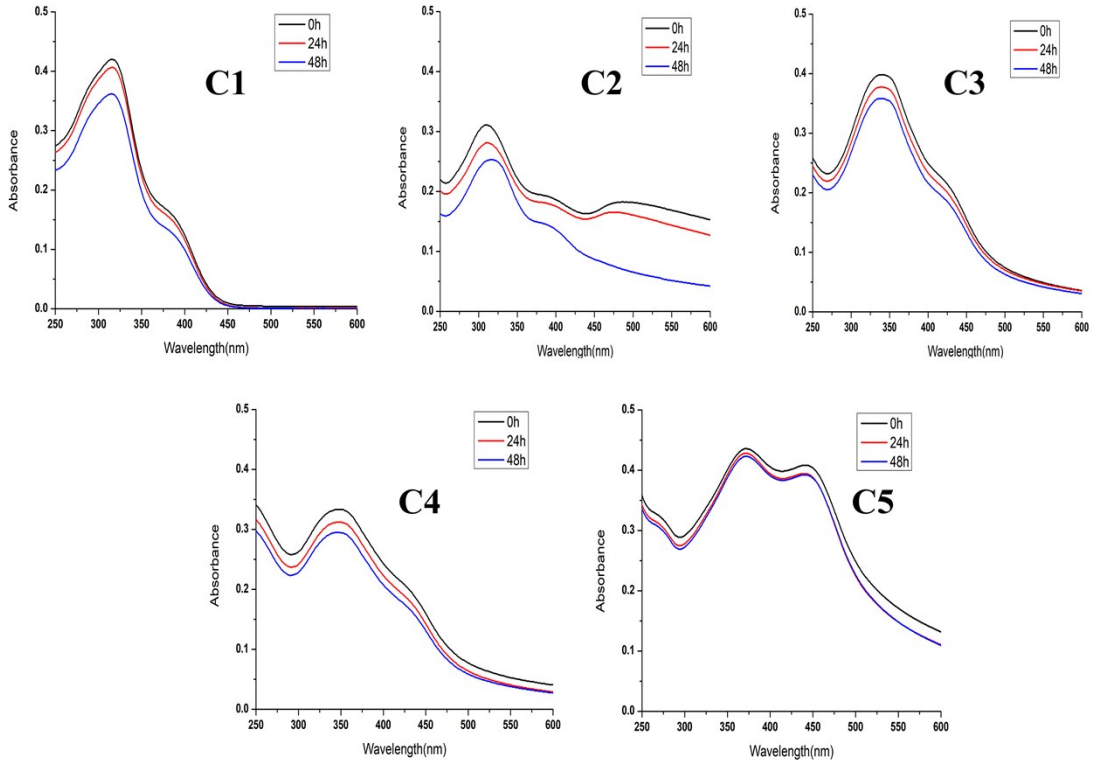

Figure S1 UV-Vis spectra of the complexes (C1-C5) in solution.

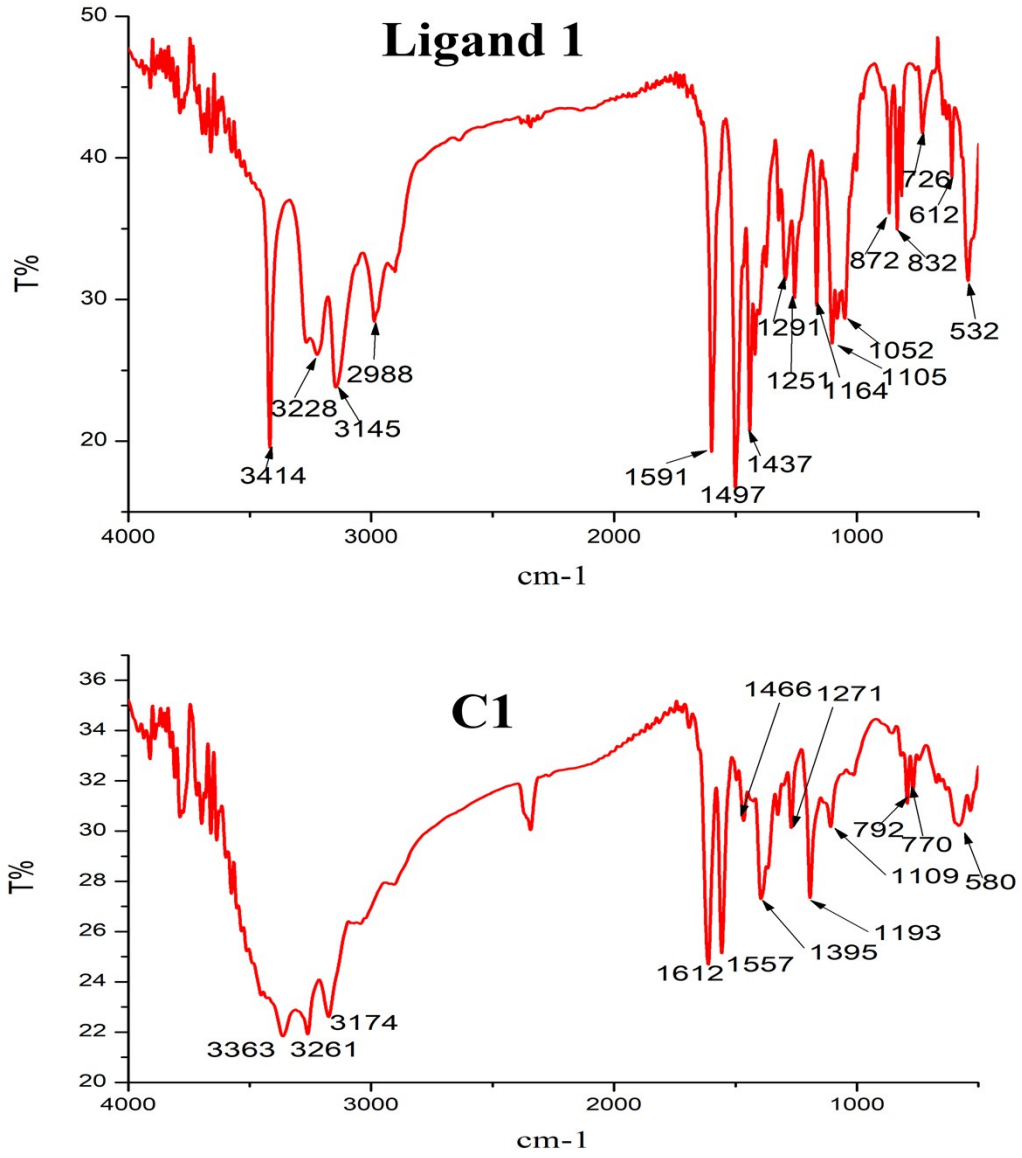

Figure S2 IR spectrum of Ligand1 and C1

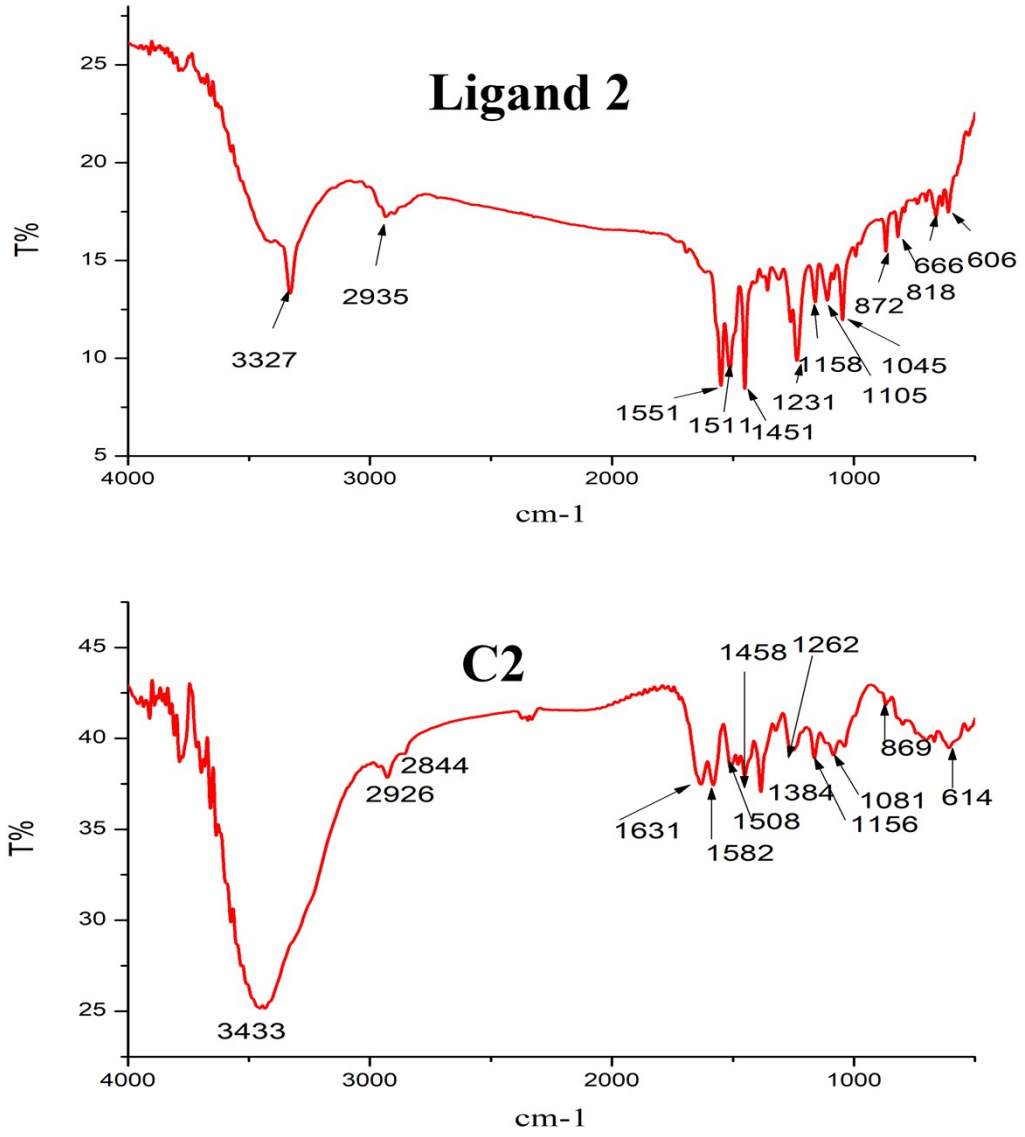

Figure S3 IR spectrum of Ligand2 and C2

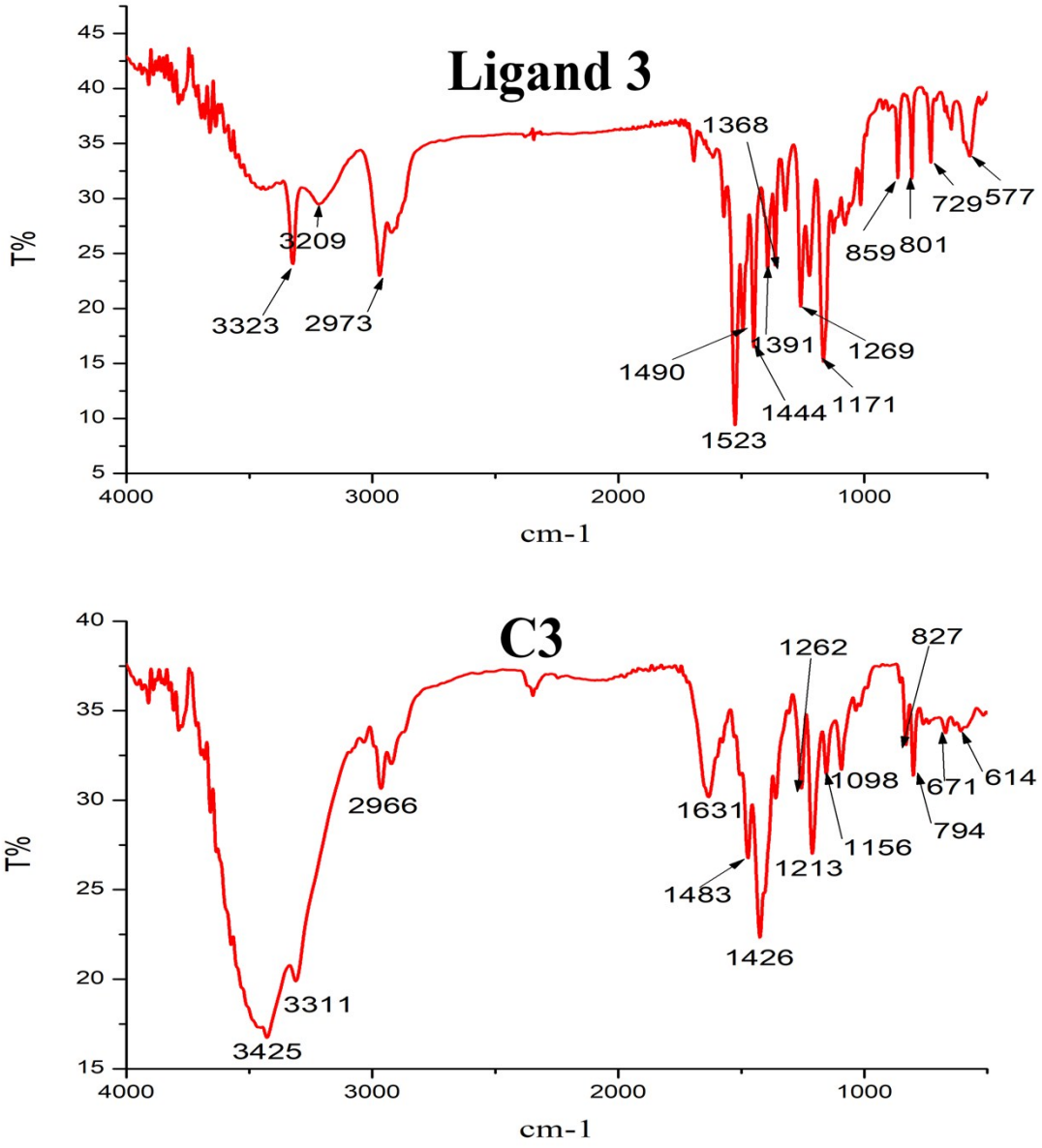

Figure S4 IR spectrum of Ligand3 and C3

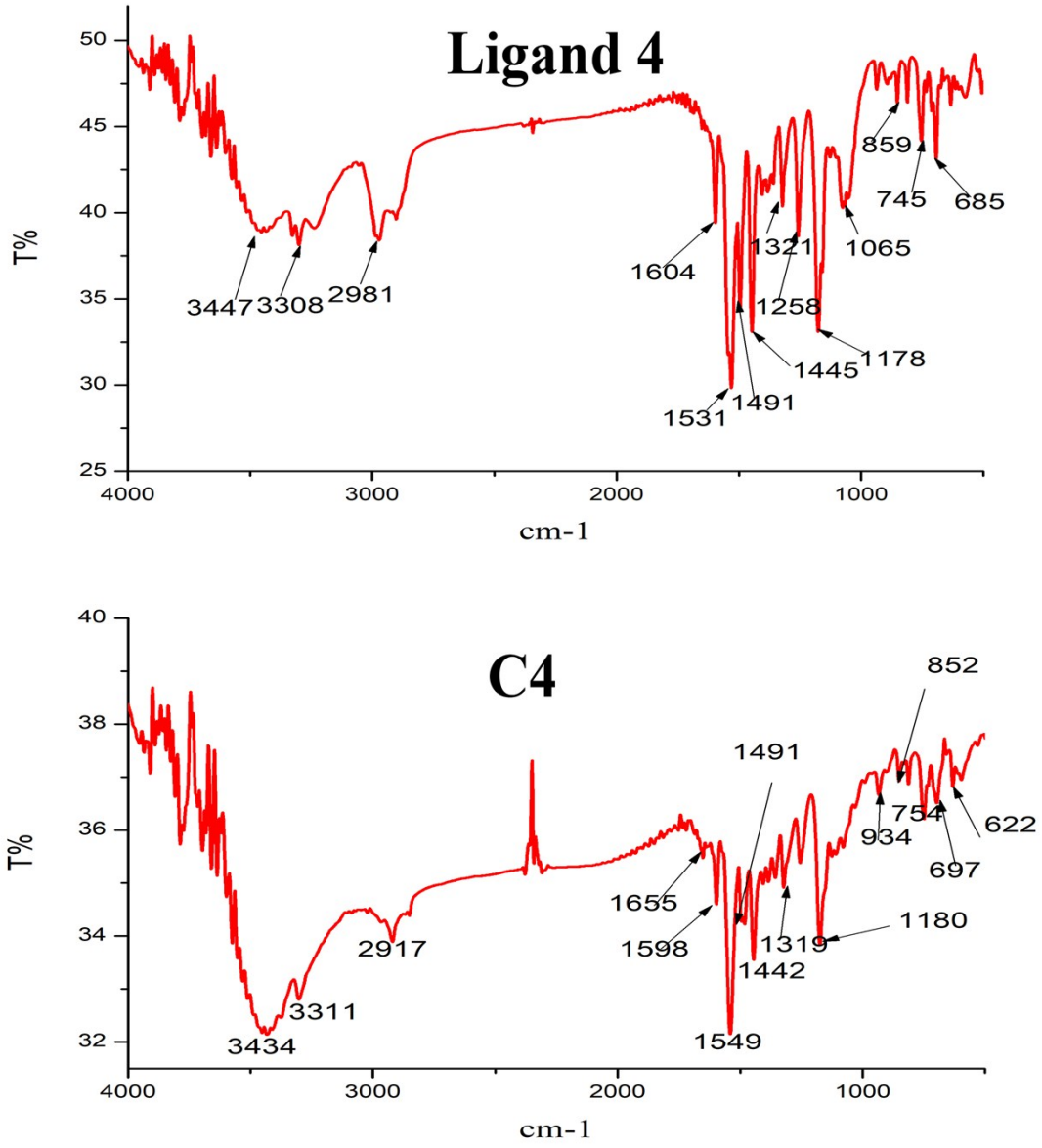

Figure S5 IR spectrum of Ligand4 and C4

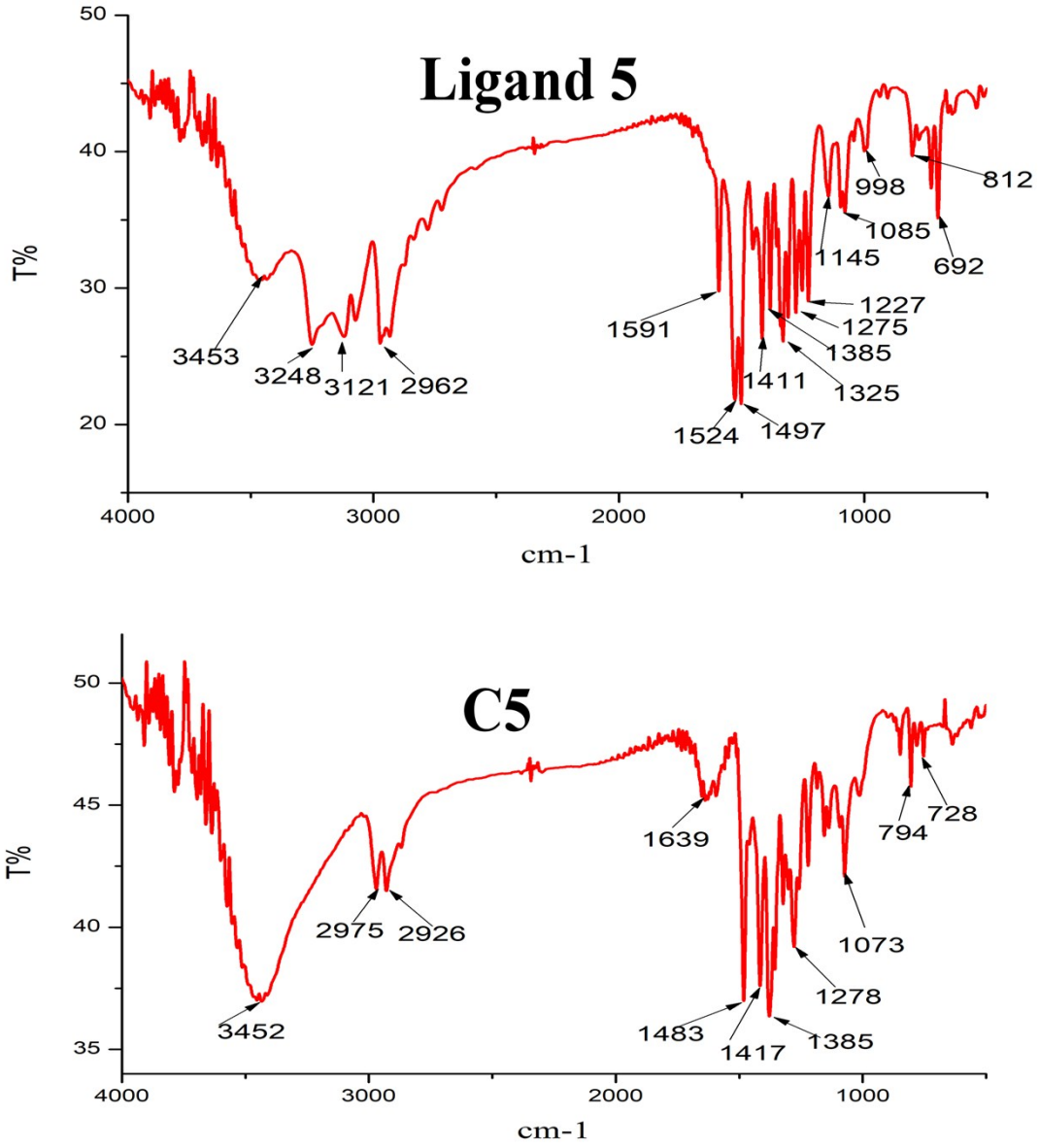

Figure S6 IR spectrum of Ligand5 and C5

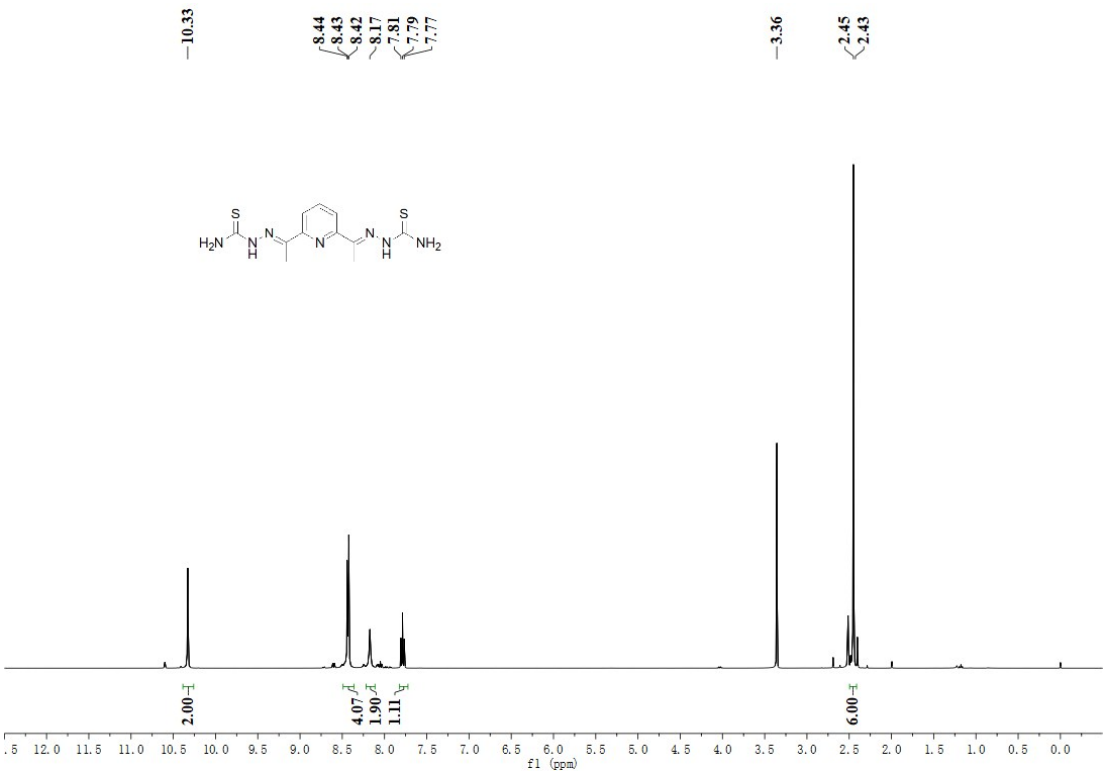

Figure S7 ^{1}H-NMR spectrum of Ligand1

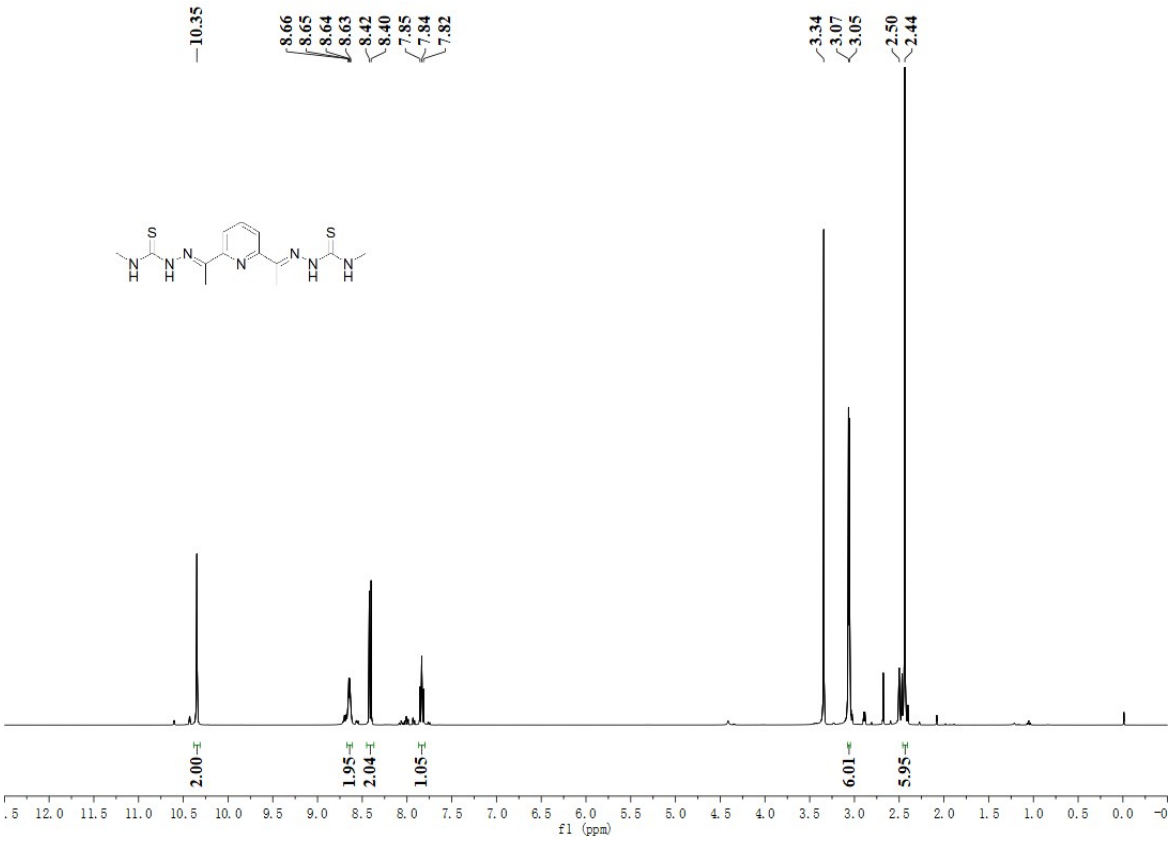

Figure S8 ^{1}H-NMR spectrum of Ligand2

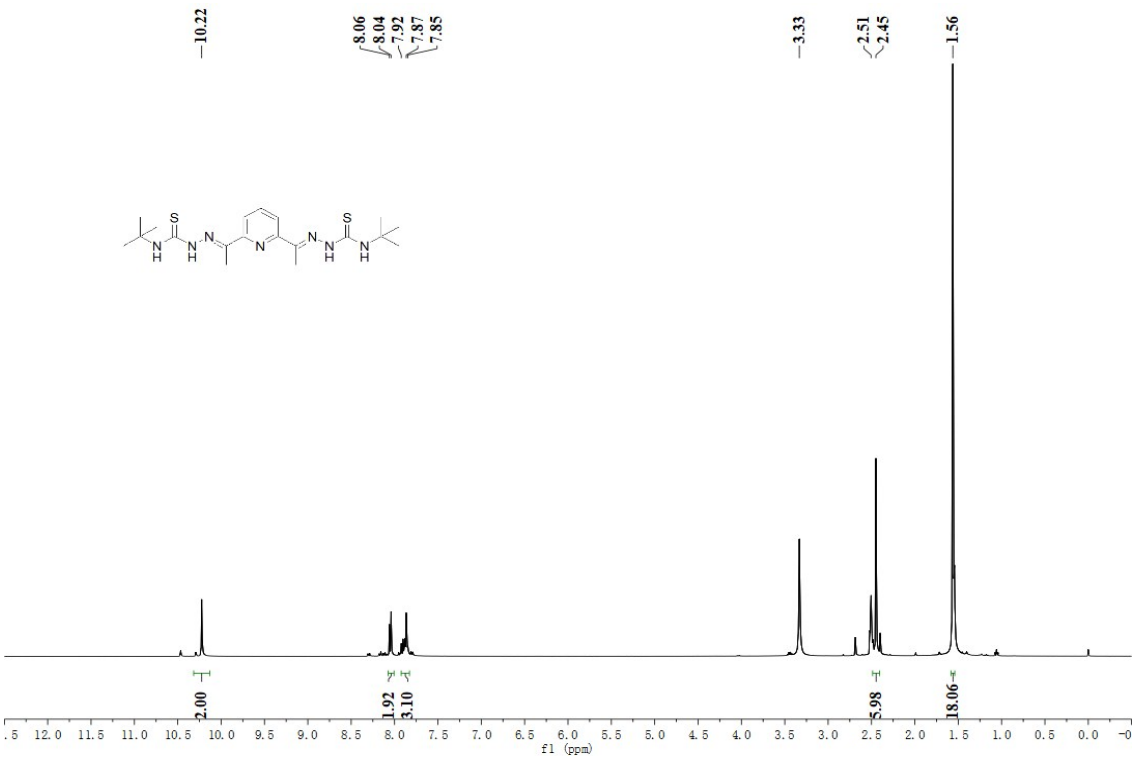

Figure S9 ^{1}H-NMR spectrum of Ligand3

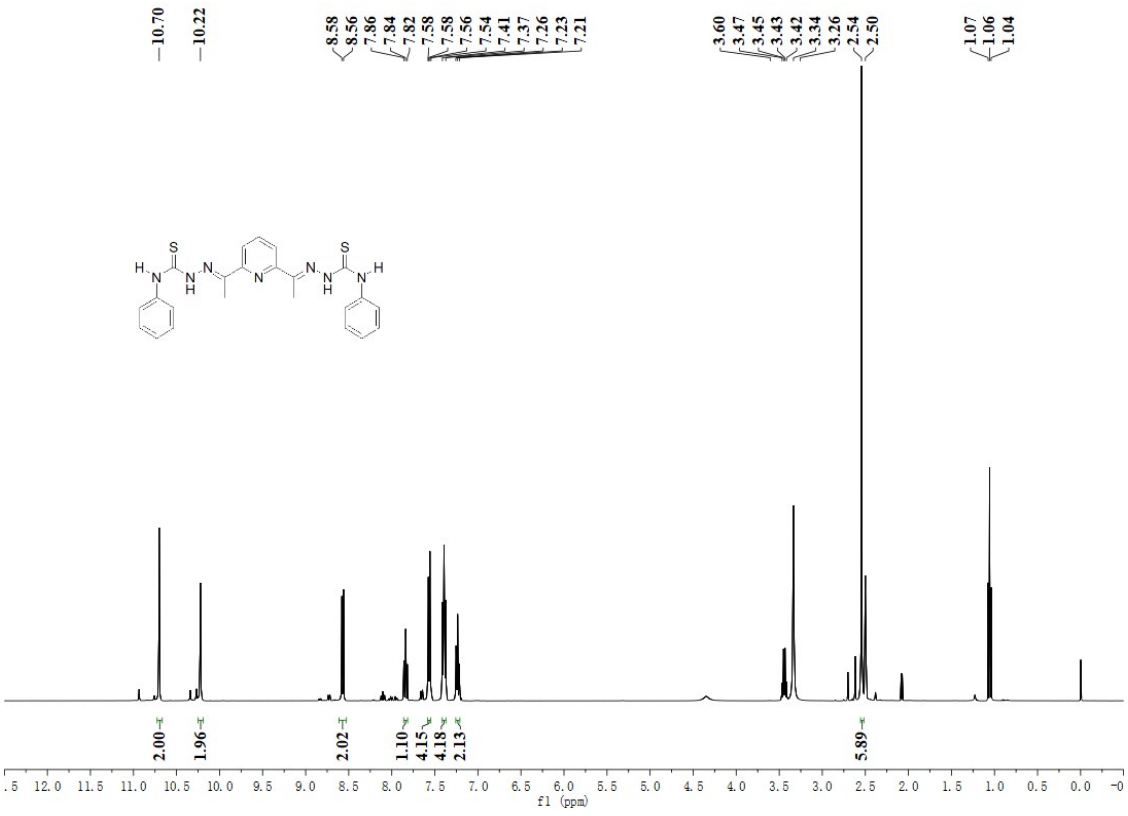

Figure S10 ^{1}H-NMR spectrum of Ligand4

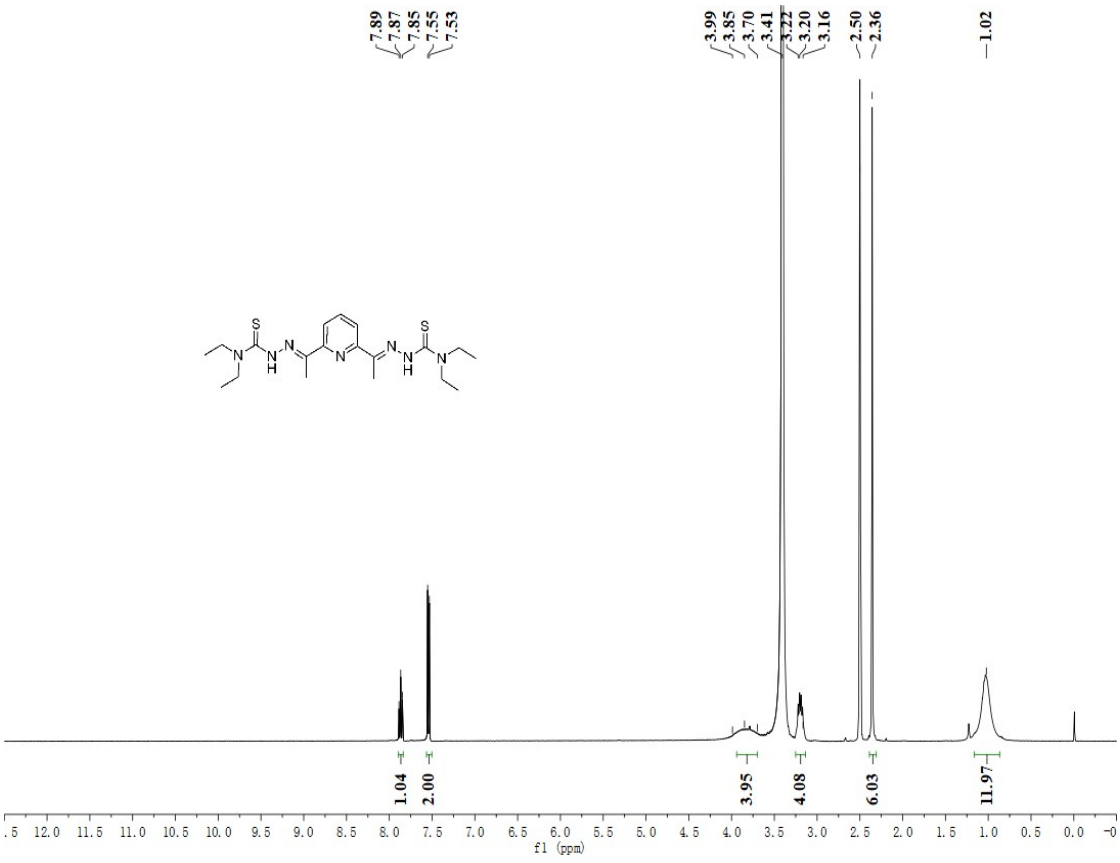

Figure S11 ^{1}H-NMR spectrum of Ligand5

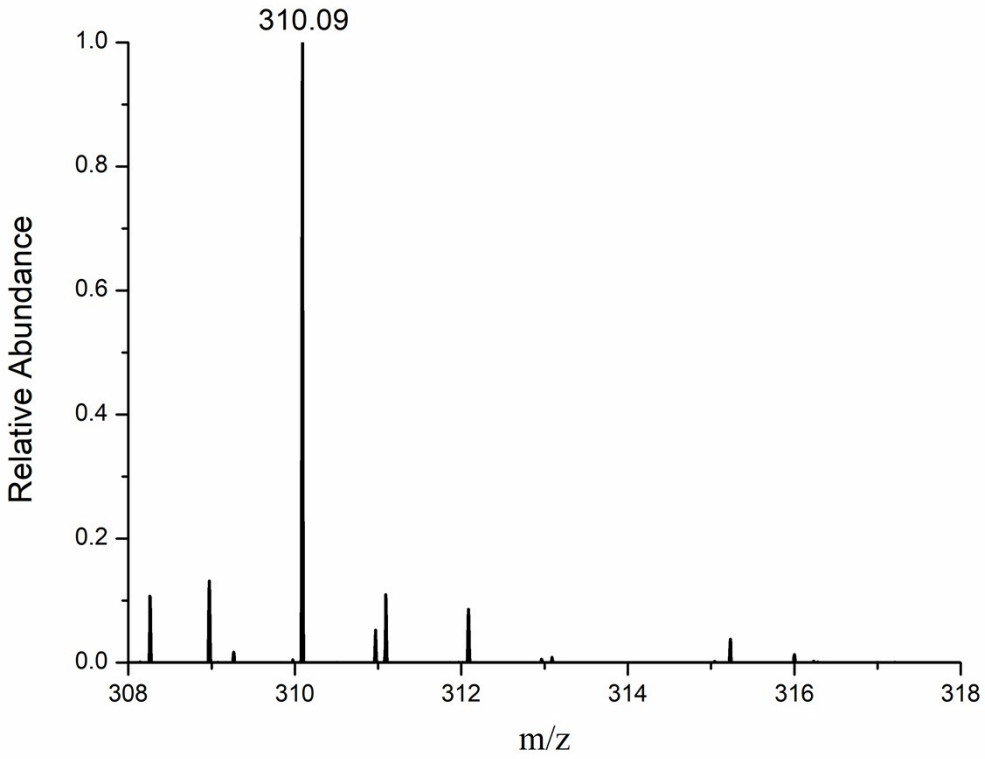

Figure S12 ESI-mass spectrum of the Ligand1showing an intense signal at m/z =310.09 for $[M+H]^+$

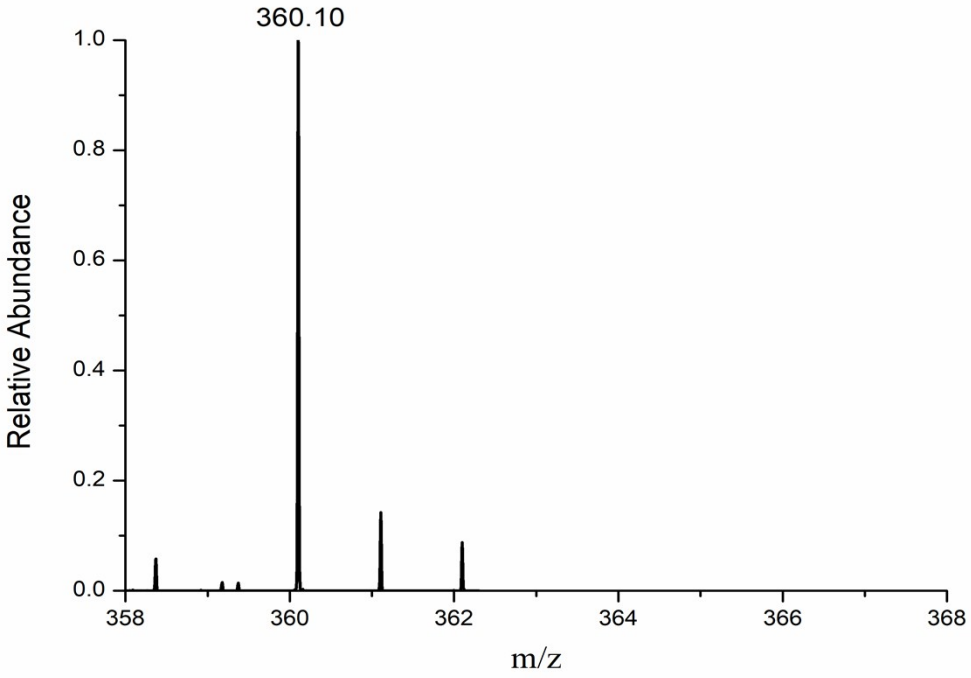

Figure S13 ESI-mass spectrum of the Ligand2 showing an intense signal at m/z=360.10 for $[M + Na]^+$

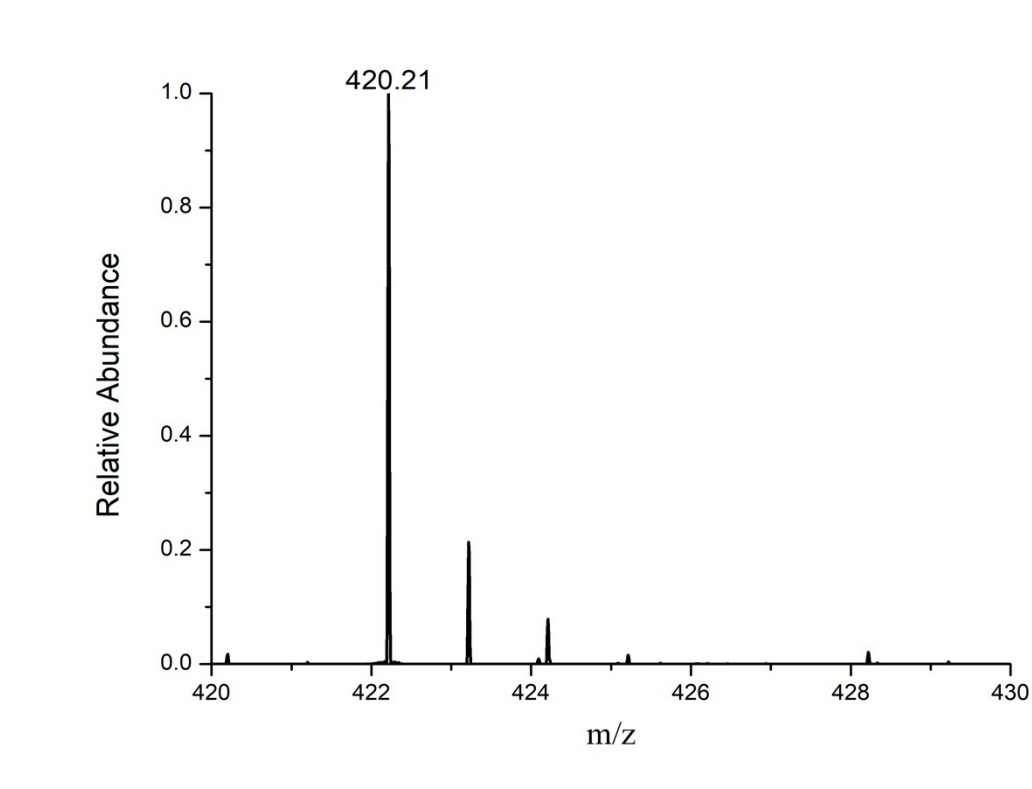

Figure S14 ESI-mass spectrum of the Ligand3 showing an intense signal at m/z=420.21 for $[M-H]^-$

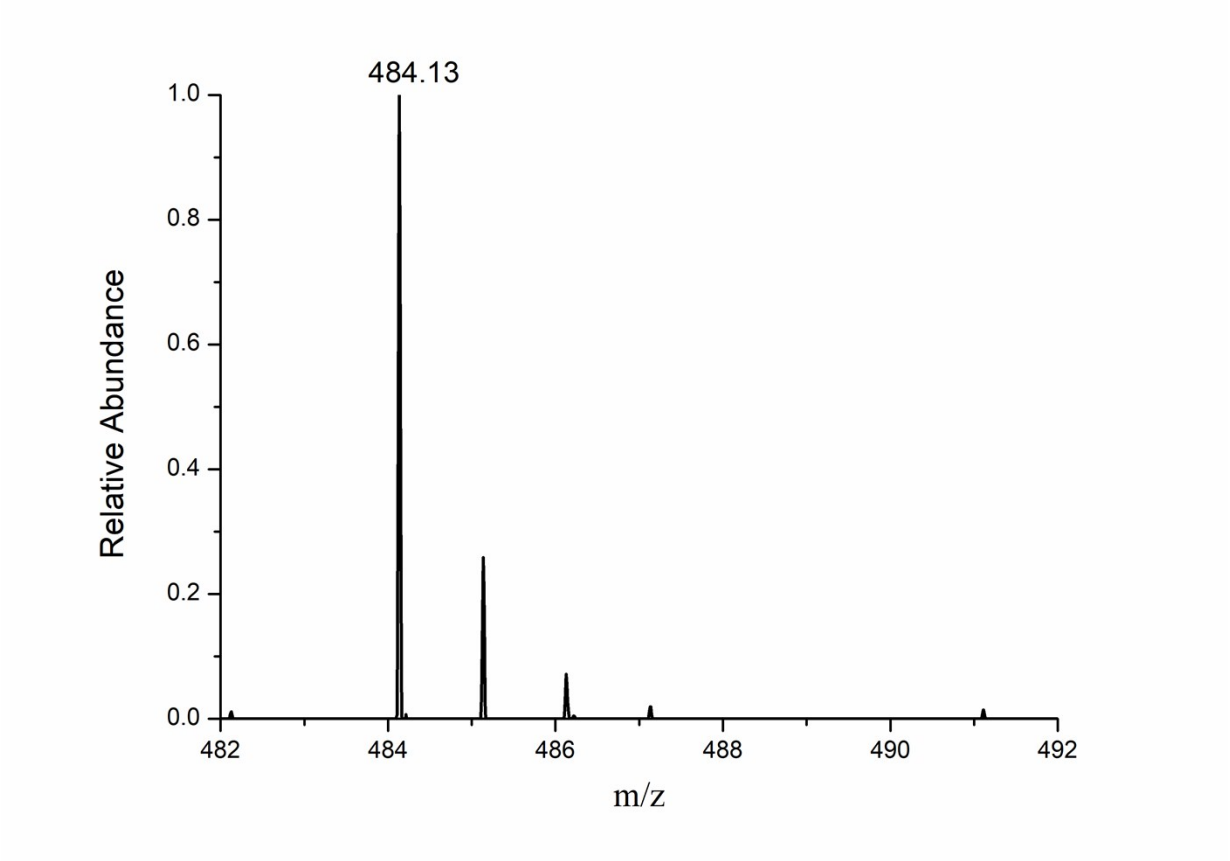

Figure S15 ESI-mass spectrum of the Ligand4 showing an intense signal at m/z=484.13 for $[M + Na]^+$

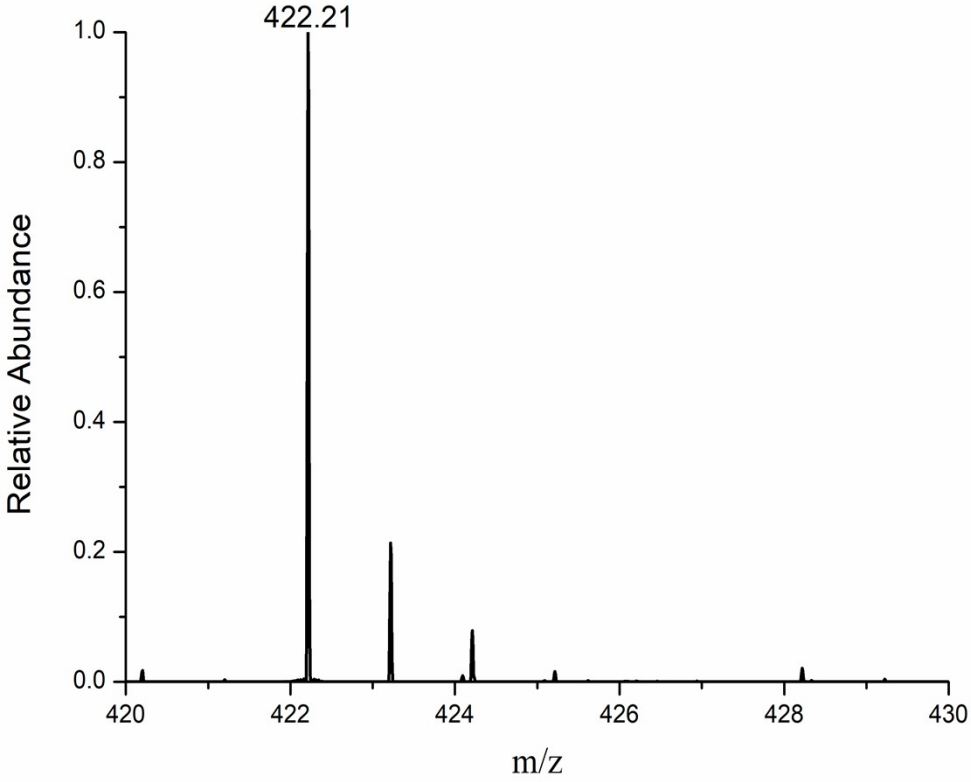

Figure S16 ESI-mass spectrum of the Ligand5 showing an intense signal at m/z=422.21 for $[M+H]^+$

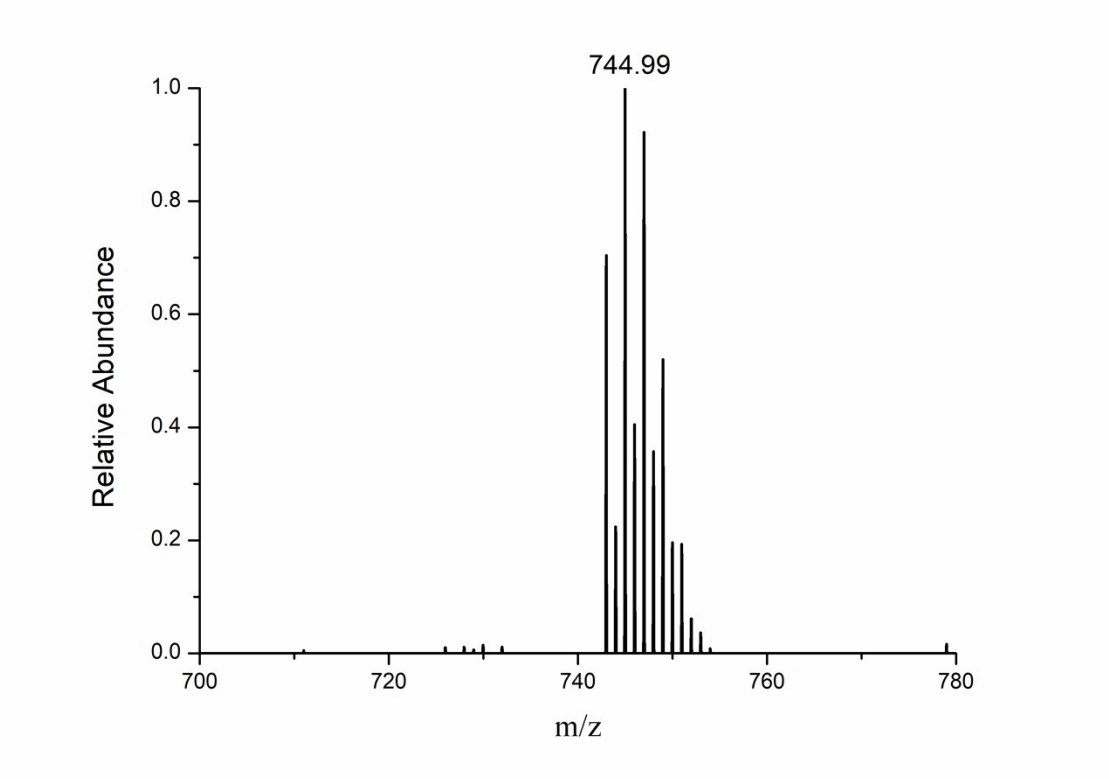

Figure S17 ESI-mass spectrum of the C1 showing an intense signal at m/z=744.99 for $[M + H]^+$

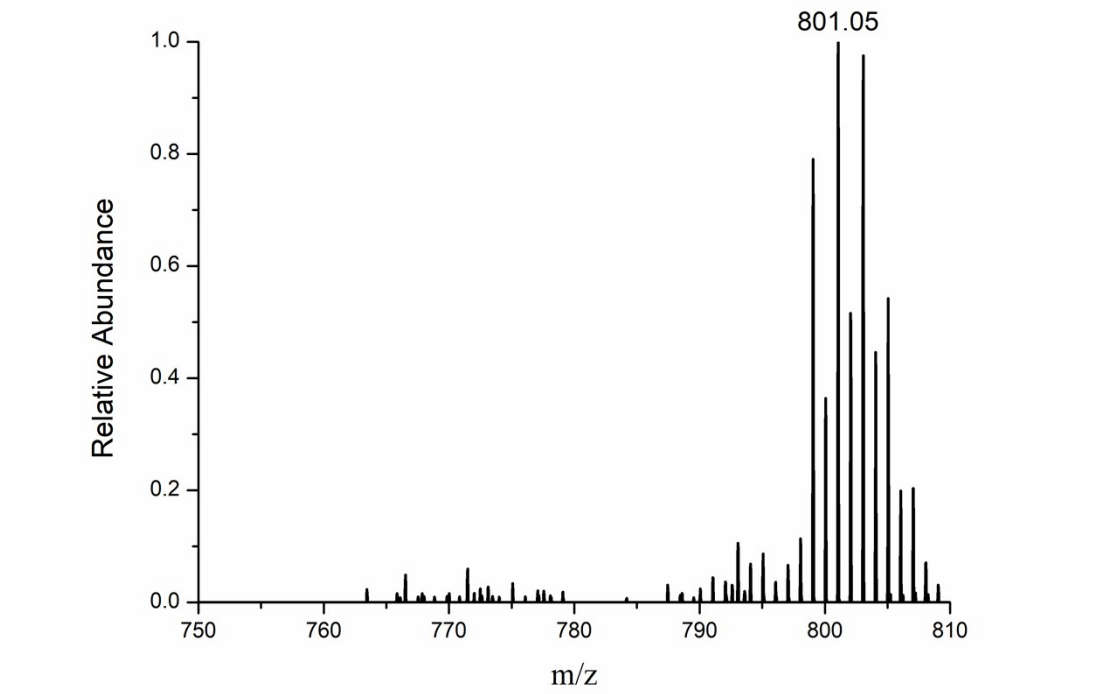

Figure S18 ESI-mass spectrum of the C2 showing an intense signal at m/z=801.05 for $[M + H]^+$

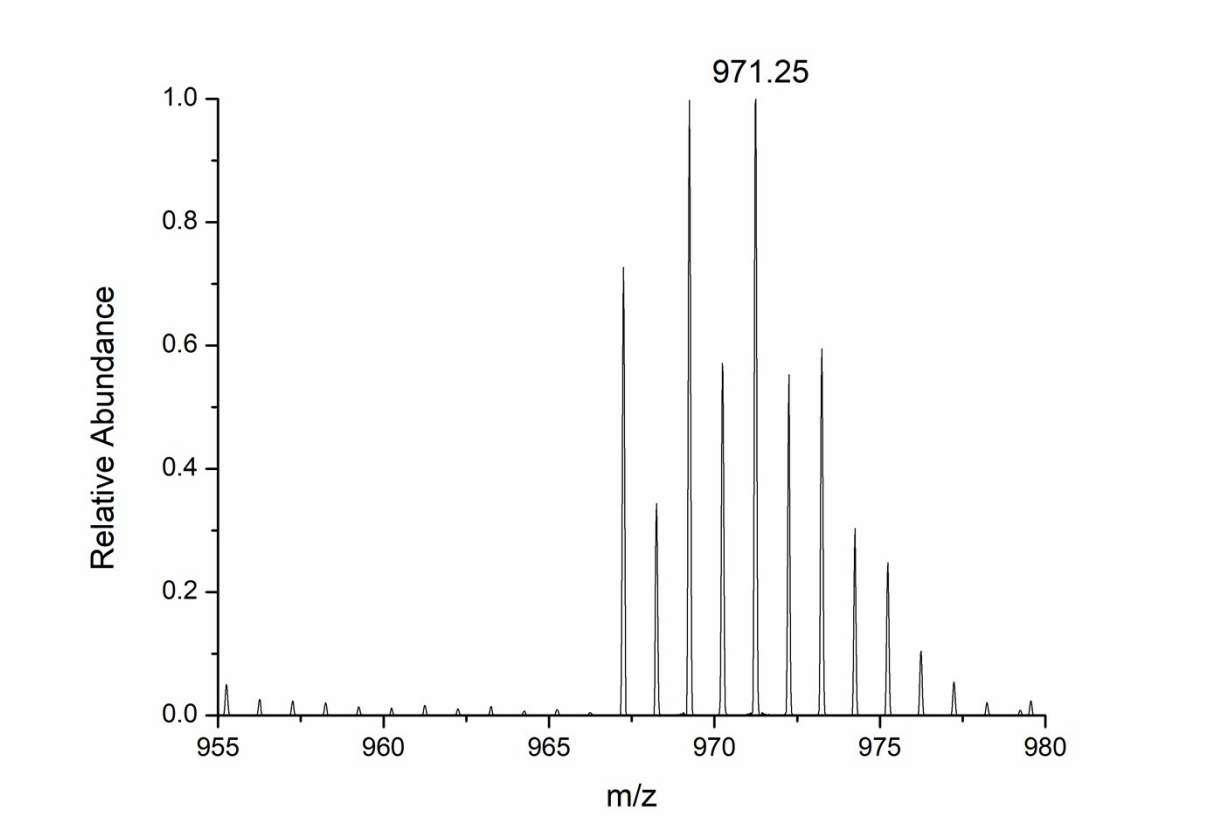

Figure S19 ESI-mass spectrum of the C3 showing an intense signal at m/z=971.25 for $[M+3H]^+$

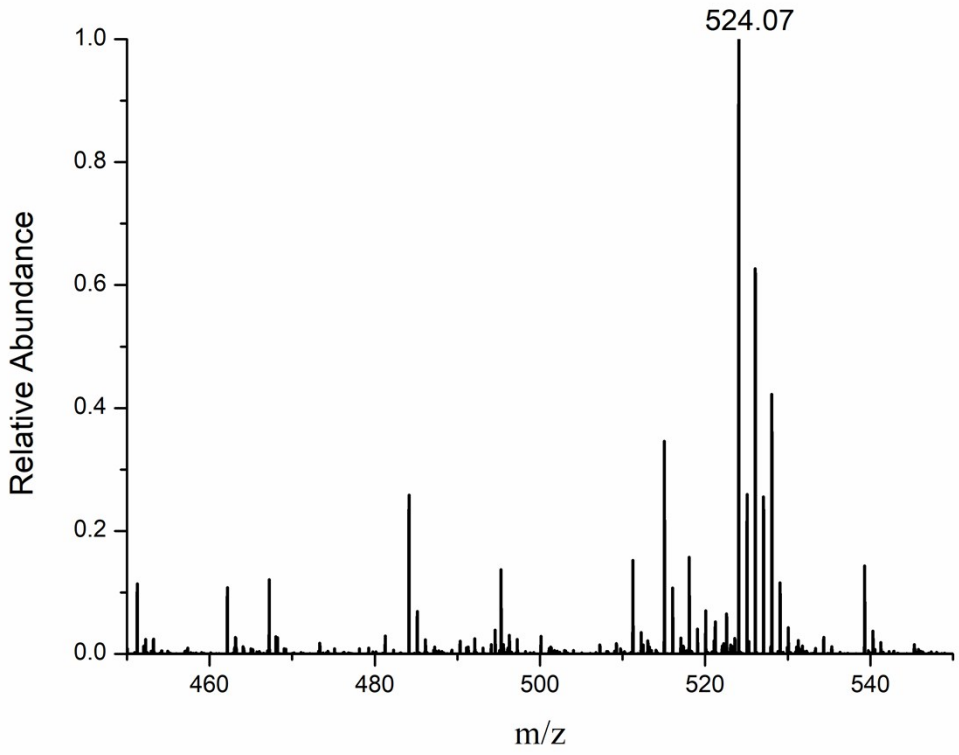

Figure S20 ESI-mass spectrum of the C4 showing an intense signal at m/z=524.07 for $[M - Cl]^+$.

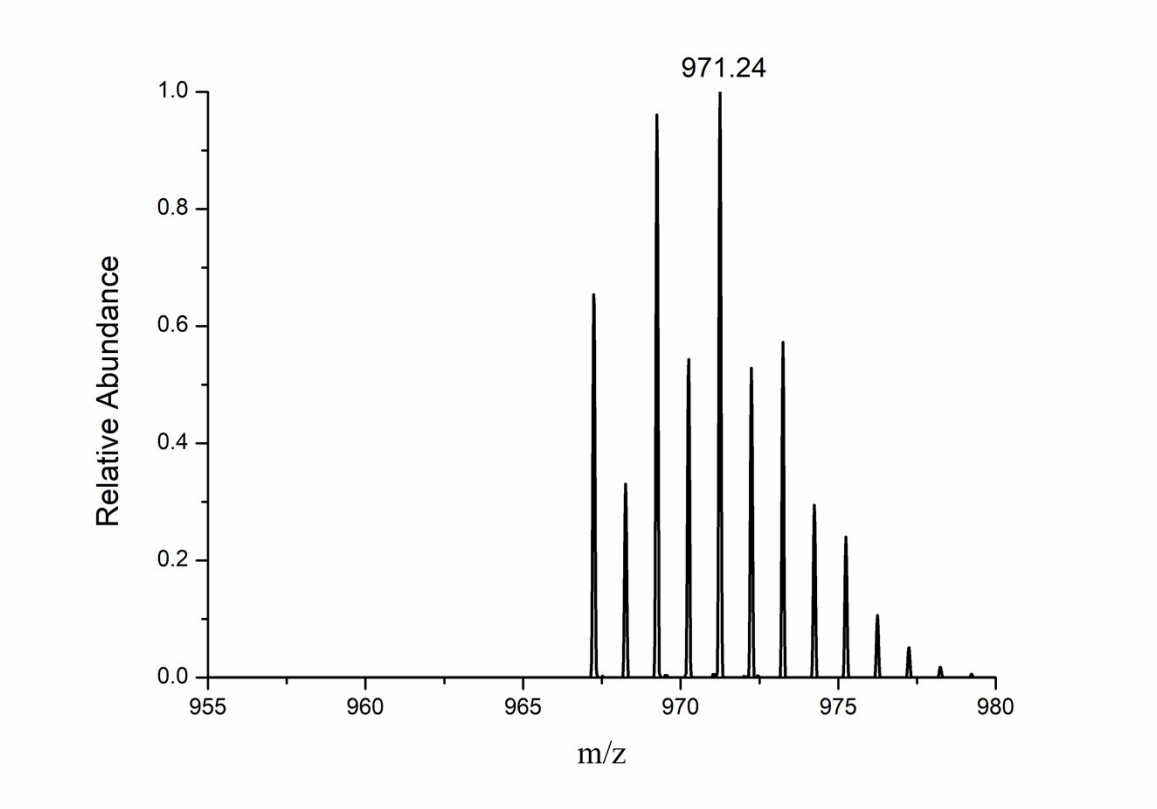

Figure S21 ESI-mass spectrum of the C4 showing an intense signal at m/z=971.24 for $[M + 3H]^+$

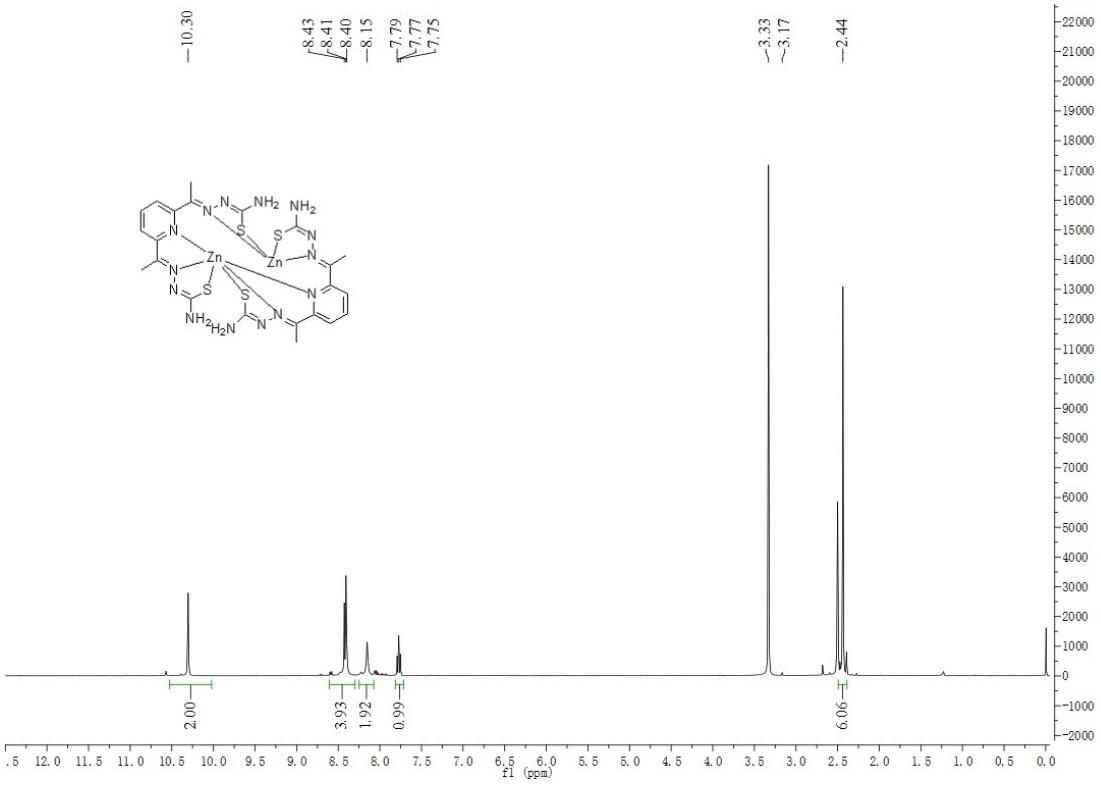

Figure S22 ^{1}H-NMR spectrum of C1

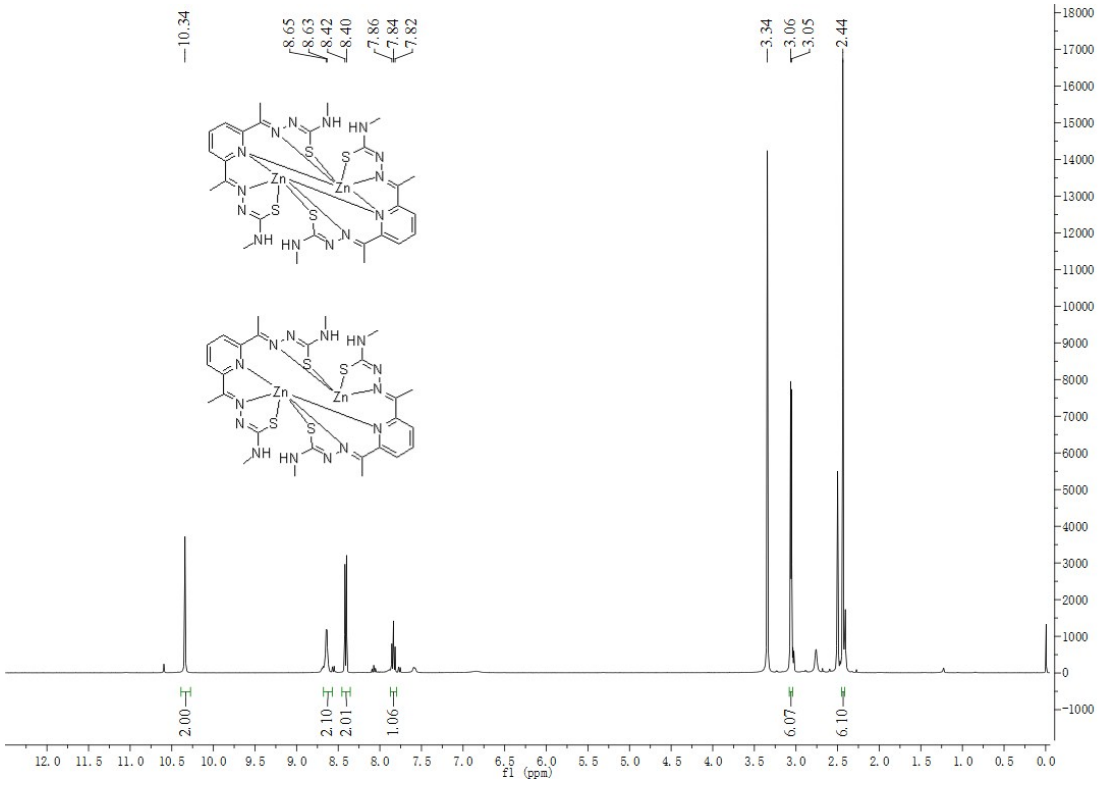

Figure S23 ^{1}H-NMR spectrum of C2

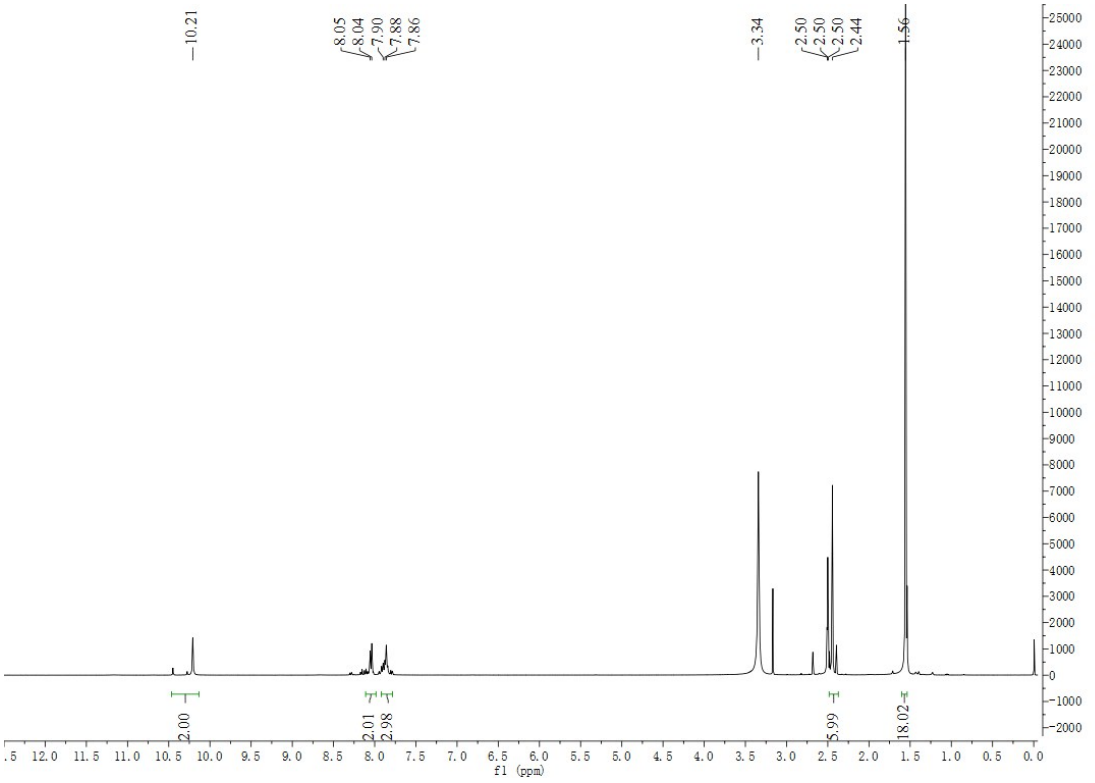

Figure S24 ^{1}H-NMR spectrum of C3

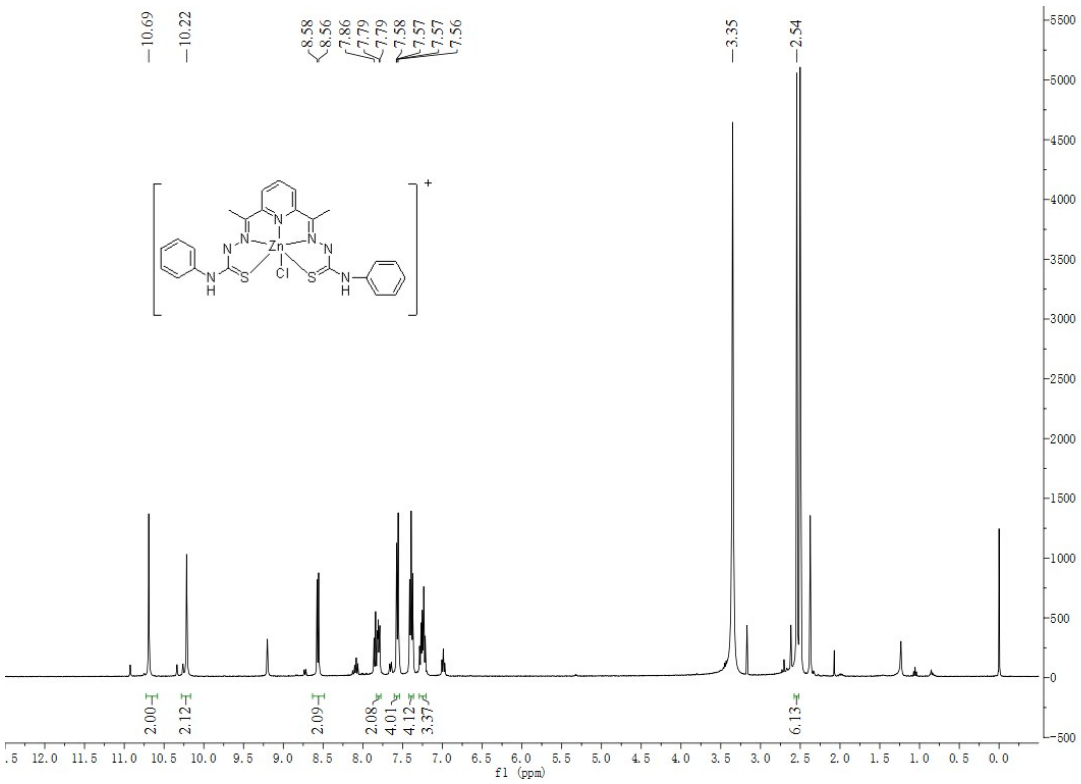

Figure S25 ^{1}H-NMR spectrum of C4

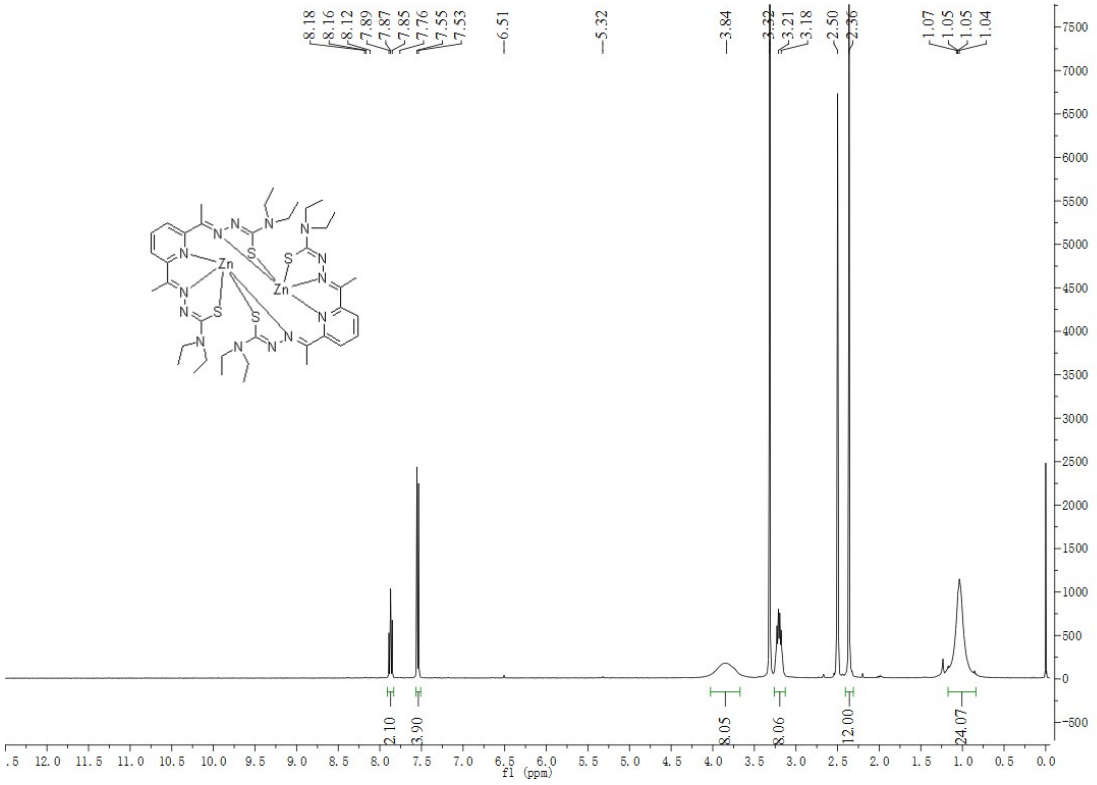

Figure S26 ^{1}H-NMR spectrum of C5

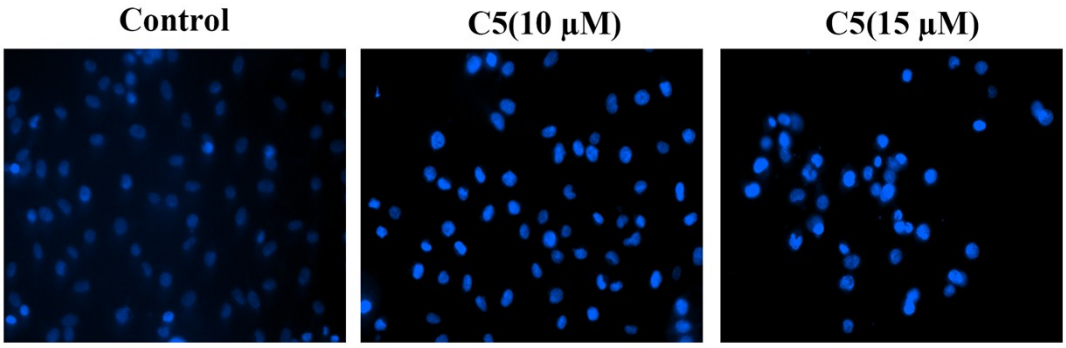

Figure S27 Morphological changes in the nuclei of cultured T-24 cells by C5 treatment. T-24 cells were treated with C5 at indicate concentration for 24 h then stained with Hoechst 33258.

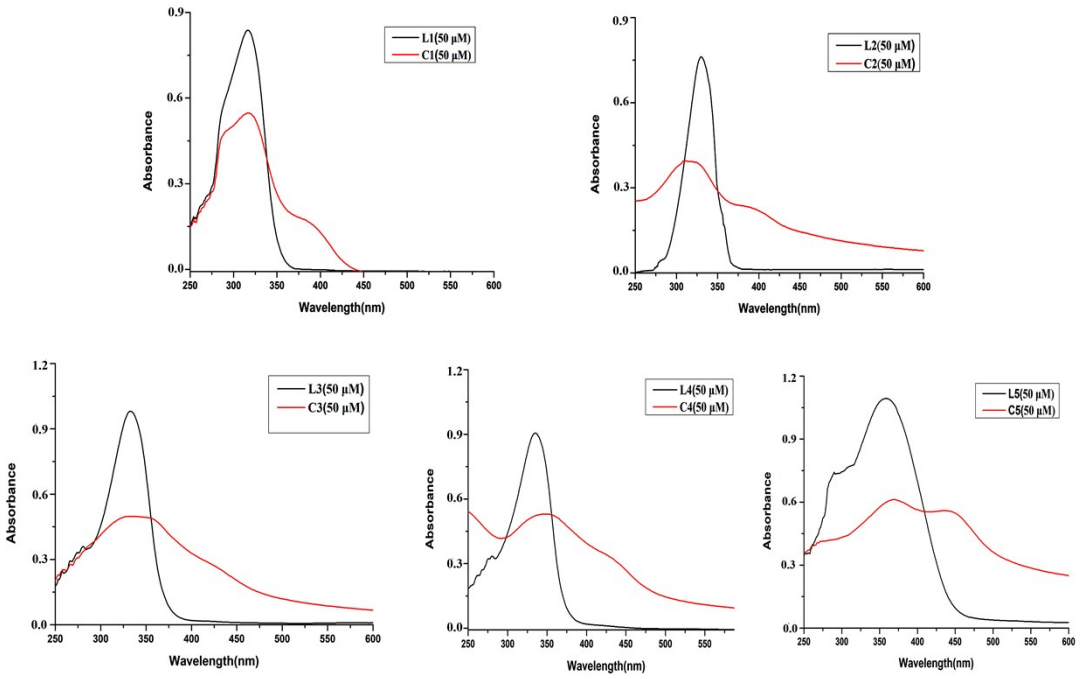

Figure S28 Absorption spectra of ligands and both zinc complexes measured in PBS.

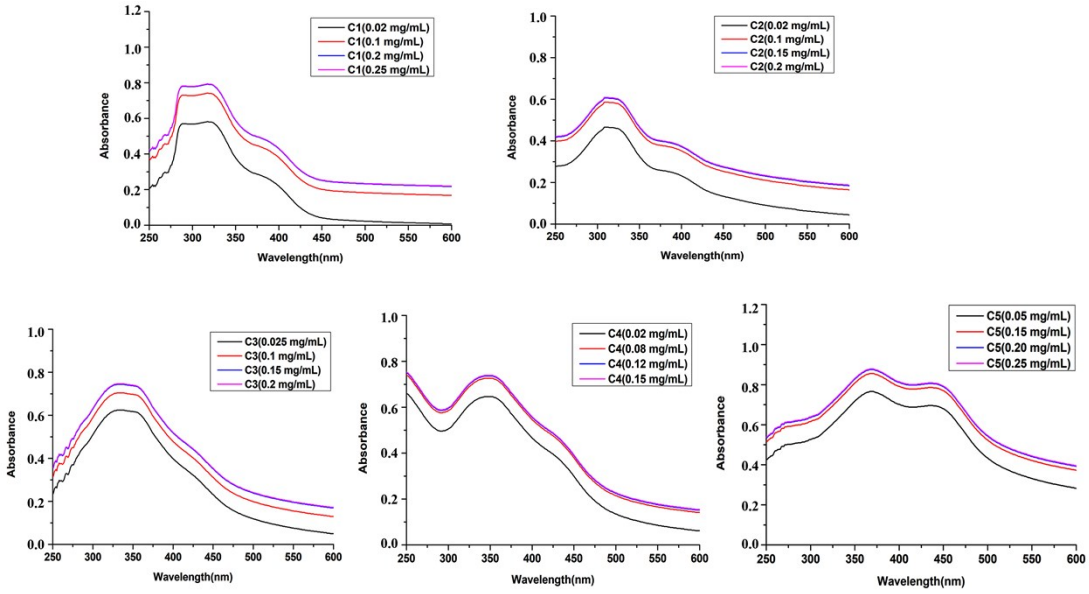

Figure S29 UV-Vis absorption spectra of C1-C5 in distilled water at room temperature, respectively