Supporting Information for

Controllable Supramolecular Structures and Luminescent Properties of Unique Trimeric Zn (II) 8-Hydroxyquinolinates Tuned by Functional Substituents

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Table of Content

1.1 Table S1. Bond lengths [Å] and angles [°] for HL_2.

N(1)-C(1)	1.3248(18)
N(1)-C(5)	1.3550(18)
C(1)-C(2)	1.4241(18)
C(1)-C(10)	1.462(2)
C(5)-C(4)	1.4198(19)
C(5)-C(6)	1.422(2)
C(11)-C(10)	1.3225(19)
C(11)-C(12)	1.462(2)
C(15)-C(16)	1.369(2)
C(15)-C(14)	1.385(2)
C(15)-N(3)	1.4635(19)
N(3)-O(5)	1.2203(19)
N(3)-O(4)	1.2213(19)
N(2)-O(2)	1.2112(18)
N(2)-O(3)	1.2163(18)
N(2)-C(17)	1.4673(18)
O(1)-C(6)	1.3576(19)
C(16)-C(17)	1.378(2)
C(17)-C(12)	1.4056(18)
C(12)-C(13)	1.403(2)
C(2)-C(3)	1.356(2)
C(6)-C(7)	1.367(2)
C(3)-C(4)	1.405(2)
C(13)-C(14)	1.370(2)
C(4)-C(9)	1.416(2)
C(9)-C(8)	1.360(3)
C(7)-C(8)	1.412(3)
C(1)-N(1)-C(5)	118.14(11)
N(1)-C(1)-C(2)	121.83(13)
N(1)-C(1)-C(10)	118.91(11)
C(2)-C(1)-C(10)	119.26(13)
N(1)-C(5)-C(4)	123.75(13)
N(1)-C(5)-C(6)	116.99(12)
C(4)-C(5)-C(6)	119.26(13)
C(10)-C(11)-C(12)	124.65(13)
C(16)-C(15)-C(14)	121.33(14)
C(16)-C(15)-N(3)	118.91(13)
C(14)-C(15)-N(3)	119.75(14)
O(5)-N(3)-O(4)	123.43(14)
O(5)-N(3)-C(15)	118.75(14)
O(4)-N(3)-C(15)	117.82(14)

O(2)-N(2)-O(3)	123.11(14)
O(2)-N(2)-C(17)	119.55(12)
O(3)-N(2)-C(17)	117.31(14)
C(15)-C(16)-C(17)	118.07(13)
C(16)-C(17)-C(12)	123.72(13)
C(16)-C(17)-N(2)	115.32(11)
C(12)-C(17)-N(2)	120.96(12)
C(13)-C(12)-C(17)	114.96(13)
C(13)-C(12)-C(11)	121.65(12)
C(17)-C(12)-C(11)	123.30(12)
C(11)-C(10)-C(1)	124.59(13)
C(3)-C(2)-C(1)	119.91(15)
O(1)-C(6)-C(7)	120.42(15)
O(1)-C(6)-C(5)	119.34(14)
C(7)-C(6)-C(5)	120.25(15)
C(2)-C(3)-C(4)	120.02(13)
C(14)-C(13)-C(12)	122.65(13)
C(3)-C(4)-C(9)	124.45(14)
C(3)-C(4)-C(5)	116.34(13)
C(9)-C(4)-C(5)	119.20(15)
C(13)-C(14)-C(15)	119.20(14)
C(8)-C(9)-C(4)	119.76(15)
C(6)-C(7)-C(8)	119.75(17)
C(9)-C(8)-C(7)	121.75(16)

1.2 Table S2. Selected bond lengths [Å] and angles [º] for 1.

Zn(1)-O(2)	2.014(2)
Zn(1)-O(1)	2.026(2)
Zn(1)-O(6)	2.171(2)
Zn(1)-N(1)	2.197(3)
Zn(1)-O(4)	2.206(3)
Zn(1)-N(2)	2.229(3)
Zn(2)-O(5)	1.969(3)
Zn(2)-O(6)	2.004(2)
Zn(2)-N(5)	2.124(4)
Zn(2)-O(1)	2.130(2)
Zn(2)-N(6)	2.208(3)
Zn(3)-O(3)	1.959(3)
Zn(3)-O(4)	2.001(2)
Zn(3)-O(2)	2.163(3)

Zn(3)-N(4)	2.182(3)
Zn(3)-N(3)	2.187(3)

O(2)-Zn(1)-O(1)	171.46(10)
O(2)-Zn(1)-O(6)	97.45(10)
O(1)-Zn(1)-O(6)	76.32(9)
O(2)-Zn(1)-N(1)	107.04(11)
O(1)-Zn(1)-N(1)	78.81(10)
O(6)-Zn(1)-N(1)	155.02(10)
O(2)-Zn(1)-O(4)	75.95(10)
O(1)-Zn(1)-O(4)	97.78(10)
O(6)-Zn(1)-O(4)	88.09(10)
N(1)-Zn(1)-O(4)	93.02(11)
O(2)-Zn(1)-N(2)	78.91(11)
O(1)-Zn(1)-N(2)	107.16(11)
O(6)-Zn(1)-N(2)	94.56(10)
N(1)-Zn(1)-N(2)	94.92(11)
O(4)-Zn(1)-N(2)	154.85(10)
O(5)-Zn(2)-O(6)	165.12(13)
O(5)-Zn(2)-N(5)	83.26(14)
O(6)-Zn(2)-N(5)	110.93(13)
O(5)-Zn(2)-O(1)	95.14(10)
O(6)-Zn(2)-O(1)	77.73(9)
N(5)-Zn(2)-O(1)	102.80(11)
O(5)-Zn(2)-N(6)	100.59(12)
O(6)-Zn(2)-N(6)	79.06(11)
N(5)-Zn(2)-N(6)	110.73(12)
O(1)-Zn(2)-N(6)	144.26(11)
O(3)-Zn(3)-O(4)	168.01(12)
O(3)-Zn(3)-O(2)	91.58(11)
O(4)-Zn(3)-O(2)	77.22(9)
O(3)-Zn(3)-N(4)	105.01(11)
O(4)-Zn(3)-N(4)	80.55(10)
O(2)-Zn(3)-N(4)	134.39(11)
O(3)-Zn(3)-N(3)	81.07(12)
O(4)-Zn(3)-N(3)	107.77(11)
O(2)-Zn(3)-N(3)	117.56(11)
N(4)-Zn(3)-N(3)	106.97(12)
C(1)-O(1)-Zn(1)	115.5(2)
C(1)-O(1)-Zn(2)	137.7(2)
Zn(1)-O(1)-Zn(2)	103.02(10)
C(18)-O(2)-Zn(1)	116.1(2)
C(18)-O(2)-Zn(3)	137.8(2)

Zn(1)-O(2)-Zn(3)	103.45(10)
C(35)-O(3)-Zn(3)	115.2(3)
C(52)-O(4)-Zn(3)	114.5(2)
C(52)-O(4)-Zn(1)	123.6(2)
Zn(3)-O(4)-Zn(1)	102.40(10)
C(69)-O(5)-Zn(2)	111.9(3)
C(86)-O(6)-Zn(2)	116.3(2)
C(86)-O(6)-Zn(1)	128.7(2)
Zn(2)-O(6)-Zn(1)	102.35(10)
C(9)-N(1)-Zn(1)	130.6(3)
C(6)-N(1)-Zn(1)	109.2(2)
C(26)-N(2)-Zn(1)	132.5(2)
C(23)-N(2)-Zn(1)	108.1(2)
C(43)-N(3)-Zn(3)	133.0(3)
C(40)-N(3)-Zn(3)	107.4(3)
C(60)-N(4)-C(57)	119.3(3)
C(60)-N(4)-Zn(3)	132.0(3)
C(57)-N(4)-Zn(3)	108.7(2)
C(77)-N(5)-Zn(2)	132.6(3)
C(74)-N(5)-Zn(2)	106.9(3)
C(94)-N(6)-Zn(2)	131.1(3)
C(91)-N(6)-Zn(2)	109.2(2)

1.3 Table S3. Selected bond lengths [Å] and angles [º] for 2.

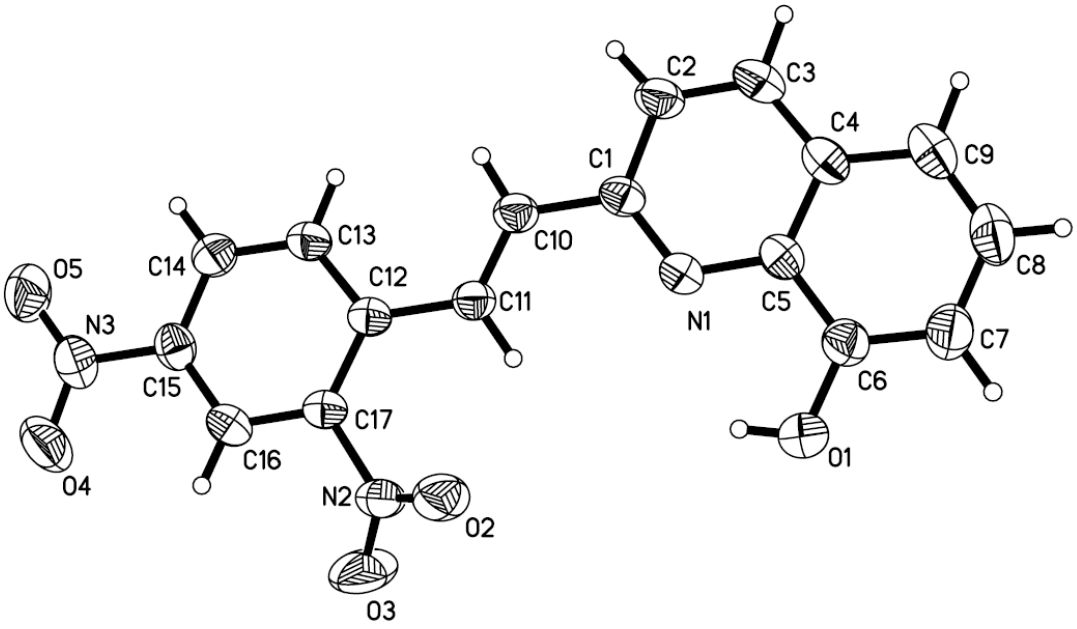
Zn(1)-O(6)	1.987(2)
Zn(1)-O(11)	2.0333(18)
Zn(1)-N(4)	2.095(3)
Zn(1)-N(7)	2.138(3)
Zn(1)-O(5)	2.145(2)
Zn(2)-O(5)	2.0106(17)
Zn(2)-O(5)#1	2.0106(17)
Zn(2)-O(11)	2.193(2)
Zn(2)-O(11)#1	2.193(2)
Zn(2)-N(3)#1	2.251(3)
Zn(2)-N(3)	2.251(3)

O(6)-Zn(1)-O(11)	159.90(9)
O(6)-Zn(1)-N(4)	83.04(10)
O(11)-Zn(1)-N(4)	115.81(9)

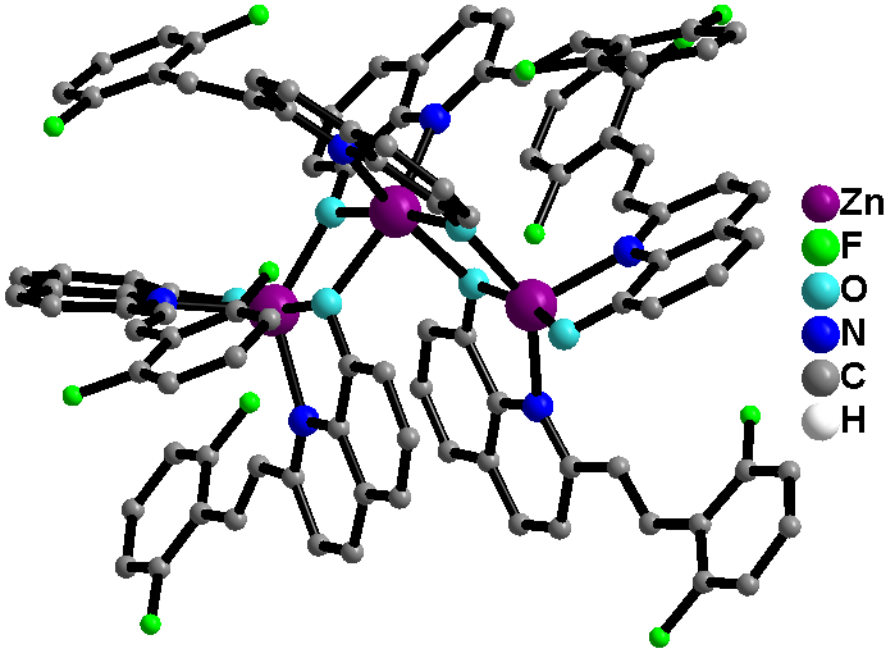
O(6)-Zn(1)-N(7)	99.15(9)
O(11)-Zn(1)-N(7)	79.99(8)
N(4)-Zn(1)-N(7)	114.30(10)
O(6)-Zn(1)-O(5)	93.31(8)
O(11)-Zn(1)-O(5)	76.81(7)
N(4)-Zn(1)-O(5)	101.30(9)
N(7)-Zn(1)-O(5)	143.35(8)
O(5)-Zn(2)-O(5)#1	170.63(13)
O(5)-Zn(2)-O(11)	76.18(8)
O(5)#1-Zn(2)-O(11)	97.17(8)
O(5)-Zn(2)-O(11)#1	97.17(8)
O(5)#1-Zn(2)-O(11)#1	76.18(8)
O(11)-Zn(2)-O(11)#1	91.34(11)
O(5)-Zn(2)-N(3)#1	108.97(9)
O(5)#1-Zn(2)-N(3)#1	78.12(8)
O(11)-Zn(2)-N(3)#1	97.06(8)
O(11)#1-Zn(2)-N(3)#1	153.75(7)
O(5)-Zn(2)-N(3)	78.12(8)
O(5)#1-Zn(2)-N(3)	108.97(9)
O(11)-Zn(2)-N(3)	153.75(7)
O(11)#1-Zn(2)-N(3)	97.06(8)
N(3)#1-Zn(2)-N(3)	86.28(13)
C(16)-O(5)-Zn(2)	117.00(17)
C(16)-O(5)-Zn(1)	138.07(17)
Zn(2)-O(5)-Zn(1)	104.73(8)
C(18)-O(6)-Zn(1)	111.6(2)
C(35)-O(11)-Zn(1)	112.95(17)
C(35)-O(11)-Zn(2)	126.30(17)
Zn(1)-O(11)-Zn(2)	102.25(8)
C(9)-N(3)-Zn(2)	133.04(19)
C(17)-N(3)-Zn(2)	107.93(19)
C(26)-N(4)-Zn(1)	131.56(19)
C(23)-N(4)-Zn(1)	108.3(2)

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

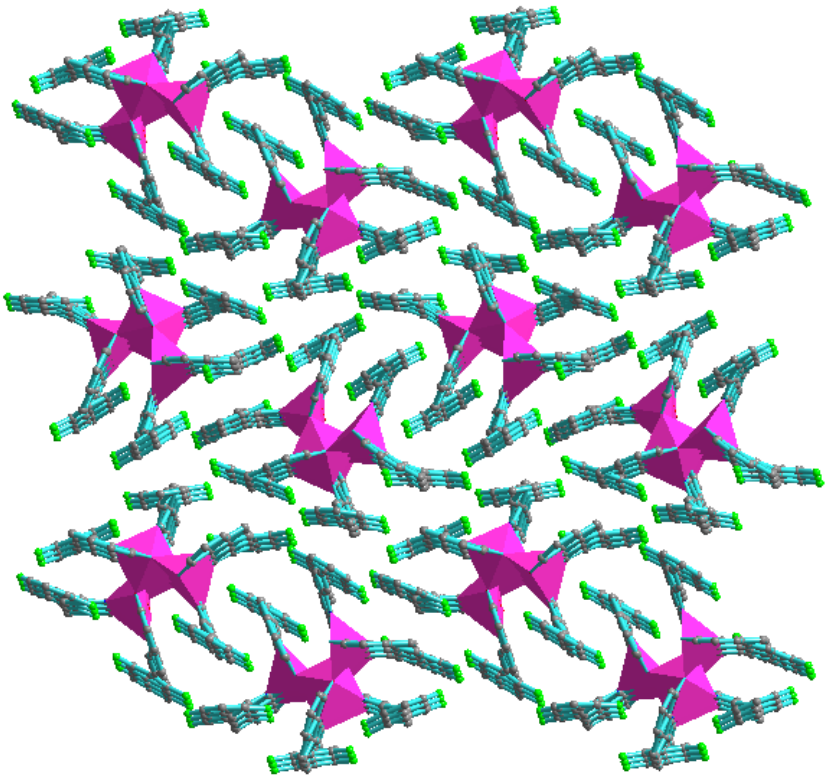
2. Figure S1. ORTEP views (at the 30% probability level) of HL_1.



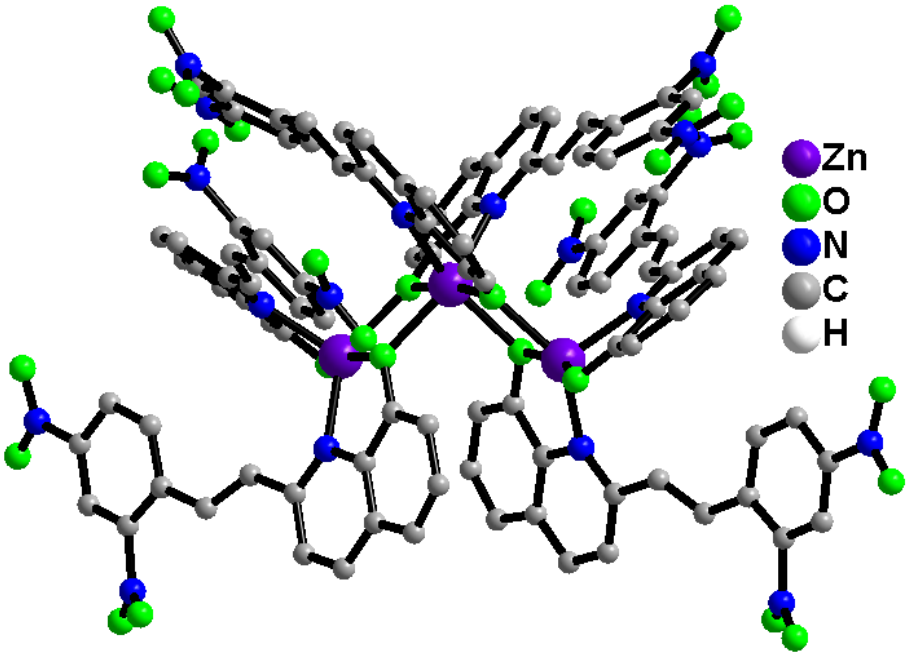
3. Figure S2. Views of the coordination geometries of Zn(II) atoms in 1.



4. Figure S3. View of 3D supramolecular structures of 1.

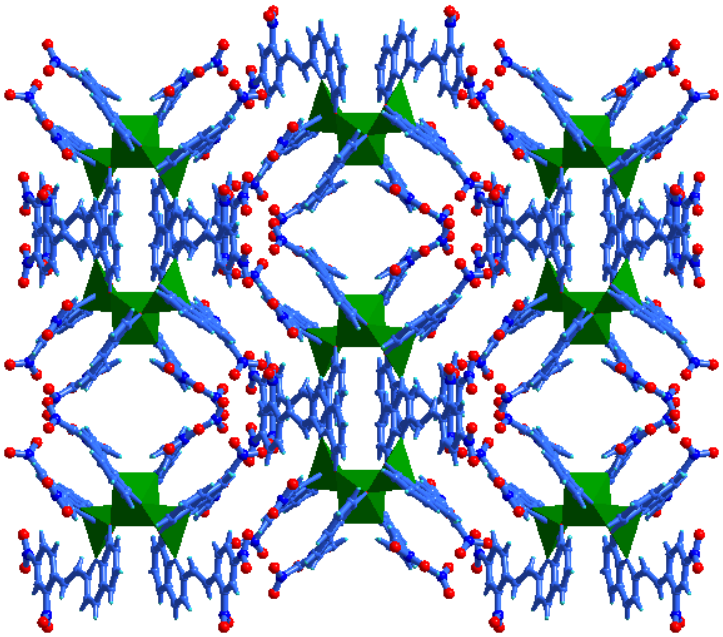


5. Figure S4. Views of the coordination geometries of Zn(II) atoms in 2.

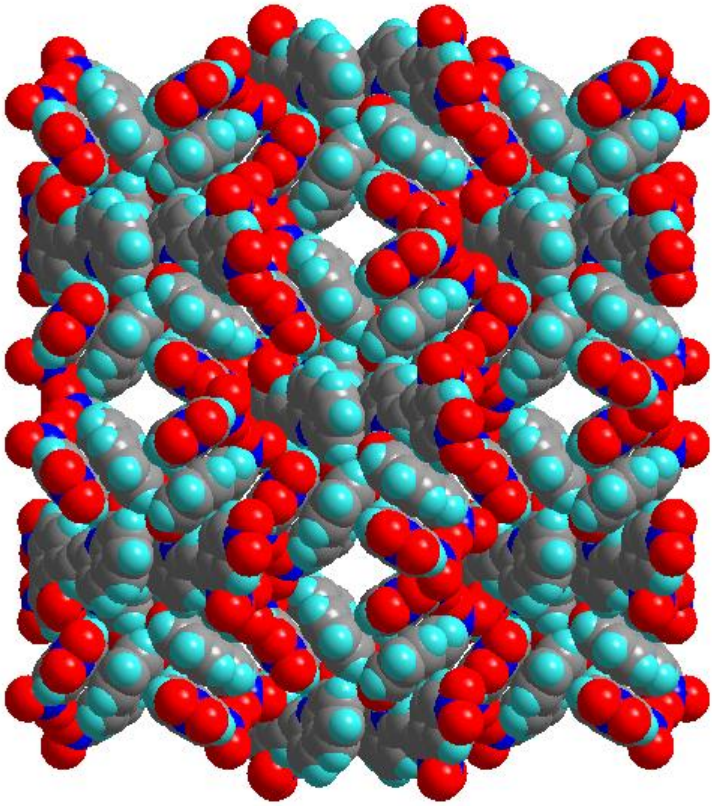


6. Figure S5. View of 3D supramolecular structures of 2.

(a):

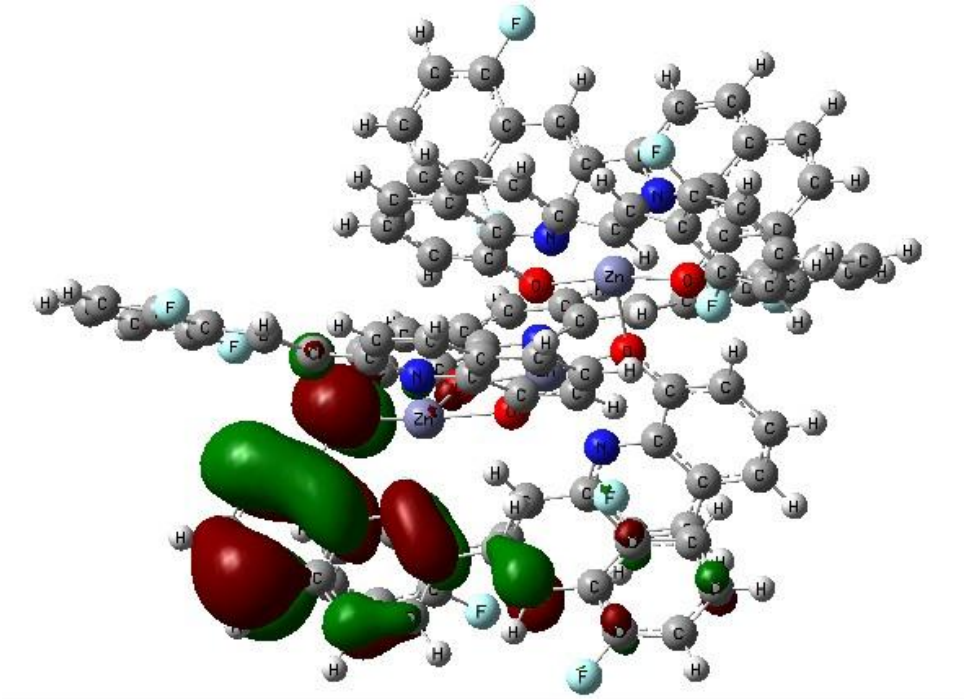


(b):

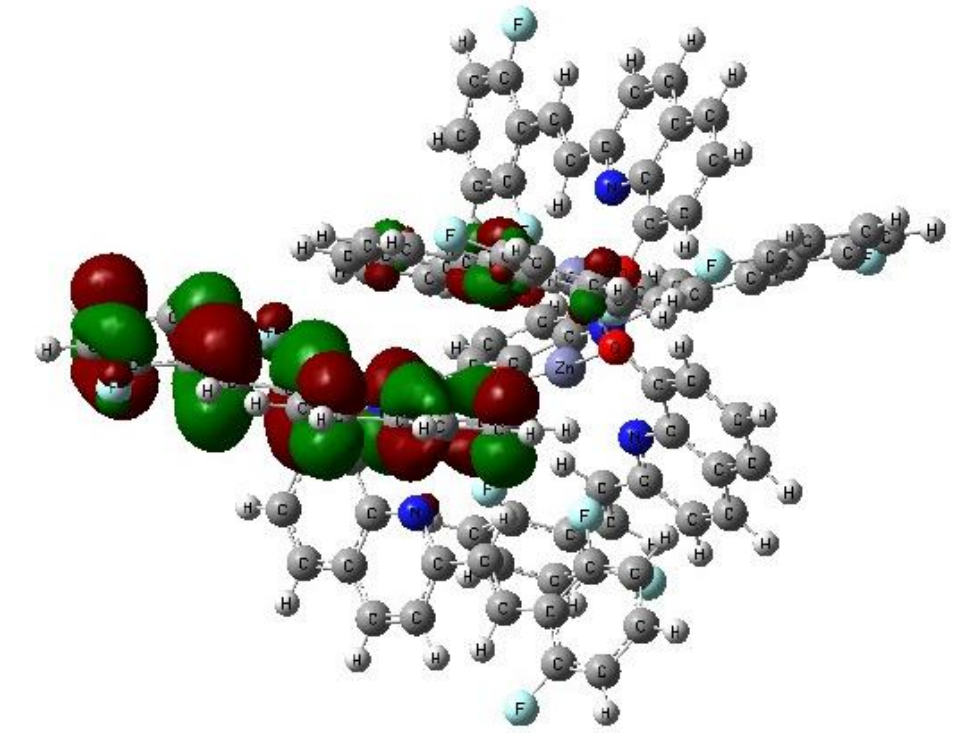


7. Figure S6. Molecular orbital amplitude plots of the (a) HOMO of the $[Zn(L_1)_2]_3$ molecule, (b) LUMO of the $[Zn(L_1)_2]_3$ molecule.

(a):

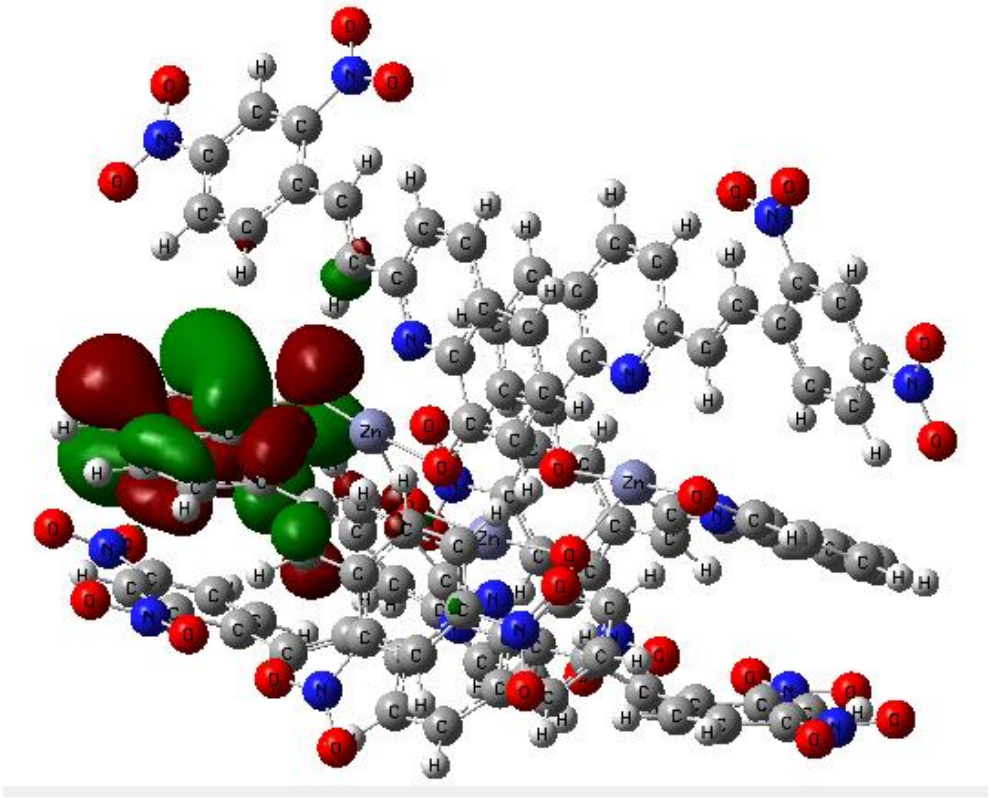


(b):

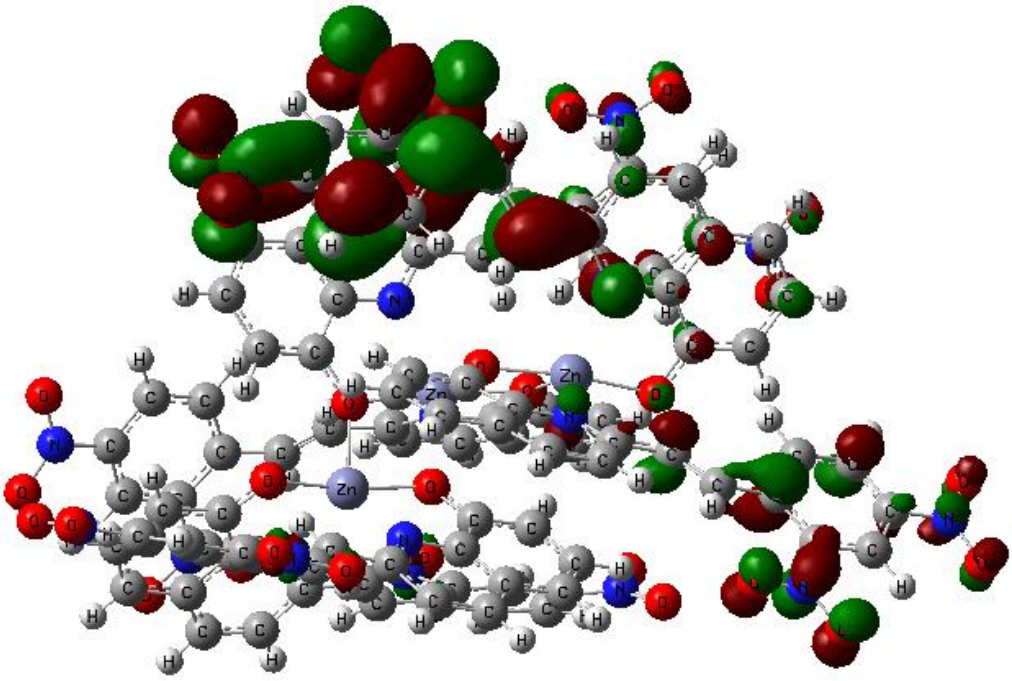


8. Figure S7. Molecular orbital amplitude plots of the (a) HOMO of the $[Zn(L_2)_2]_3$ molecule, (b) LUMO of the $[Zn(L_2)_2]_3$ molecule.

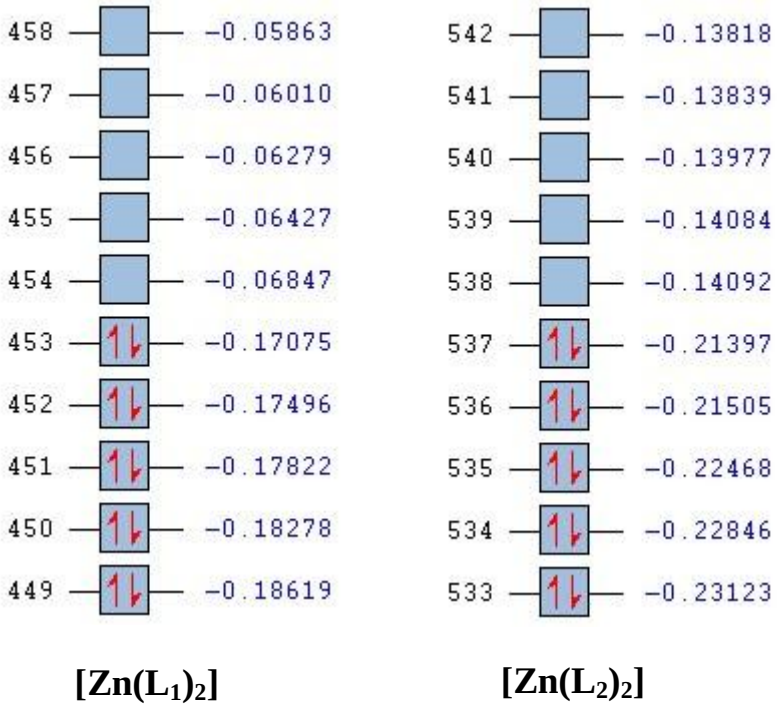
(a):



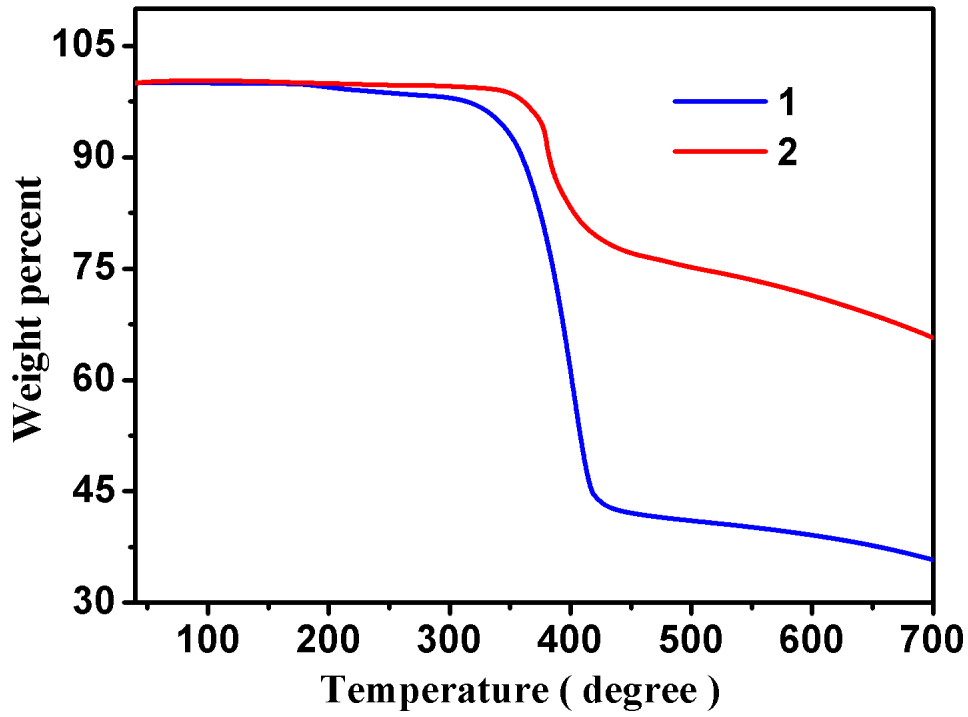
(b):



9. Figure S8. Diagram of the calculated orbital energy levels for $[Zn(L_1)_2]_3$ and $[Zn(L_2)_2]_3$ molecules.

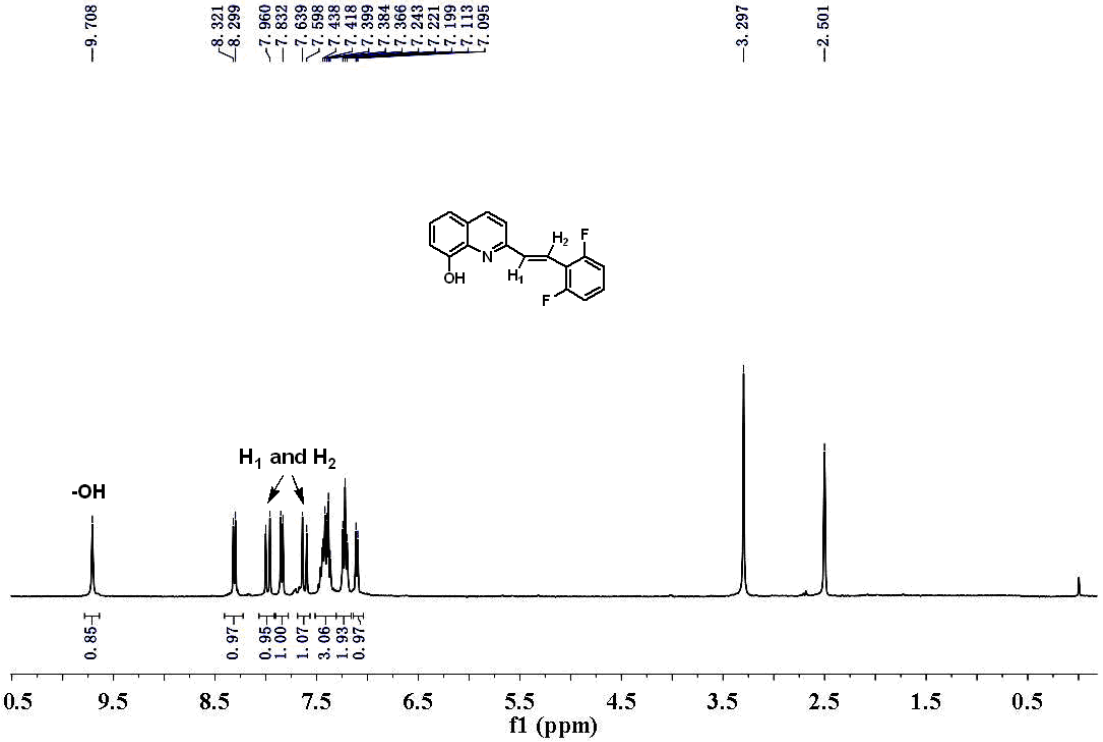


10. Figure S9. TGA curves of complexes 1 and 2.

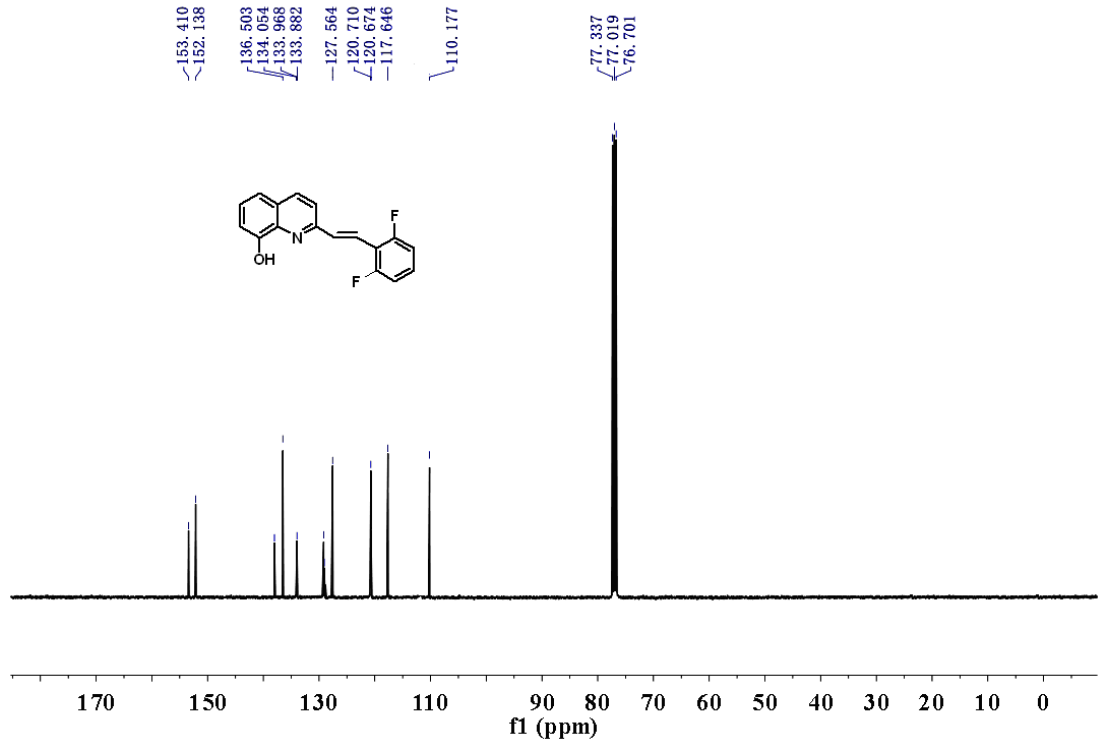


11. Figure S10. ^{1}H NMR, ^{13}C NMR spectra (d^{6}-DMSO) and ESI-MS of HL_1.

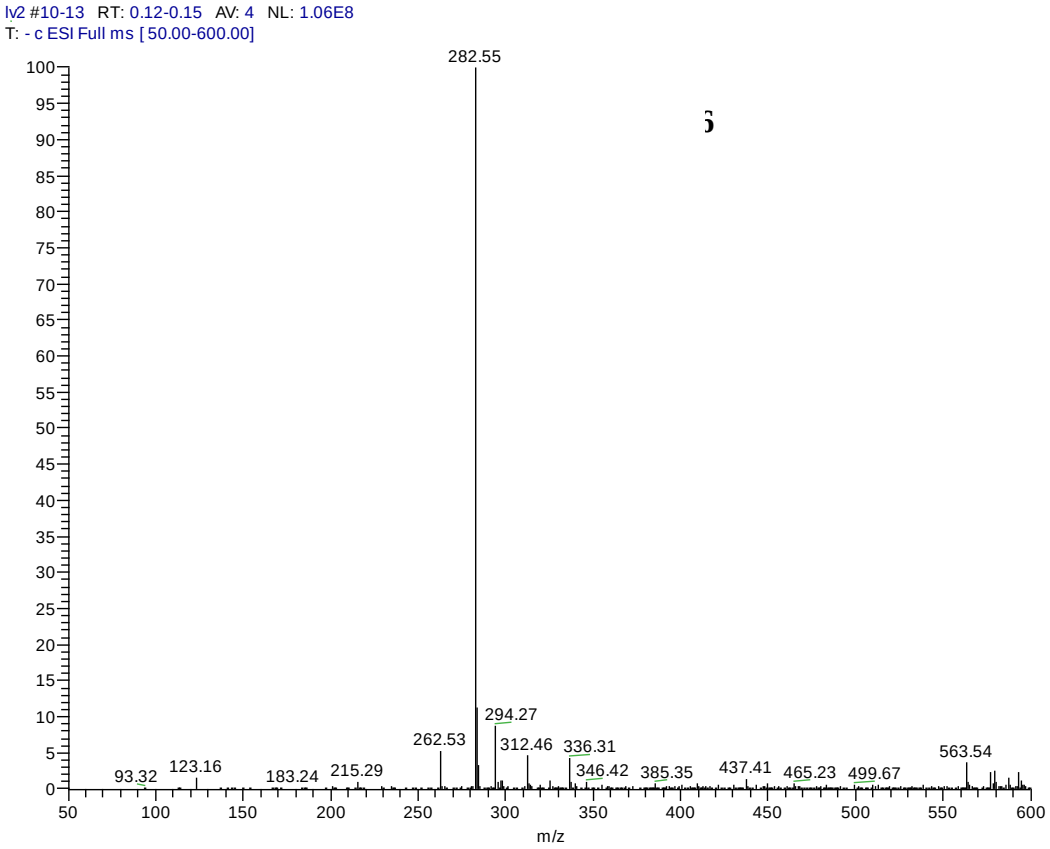
^{1}H NMR of HL_1



^{13}C NMR of HL_1

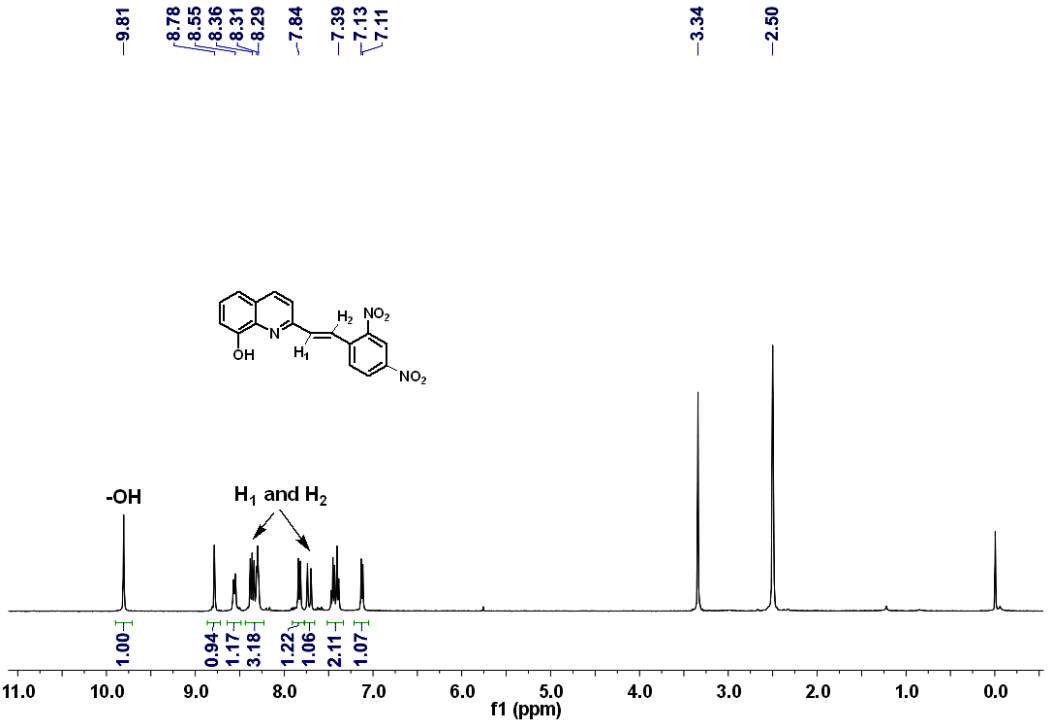


ESI-MS of HL_1

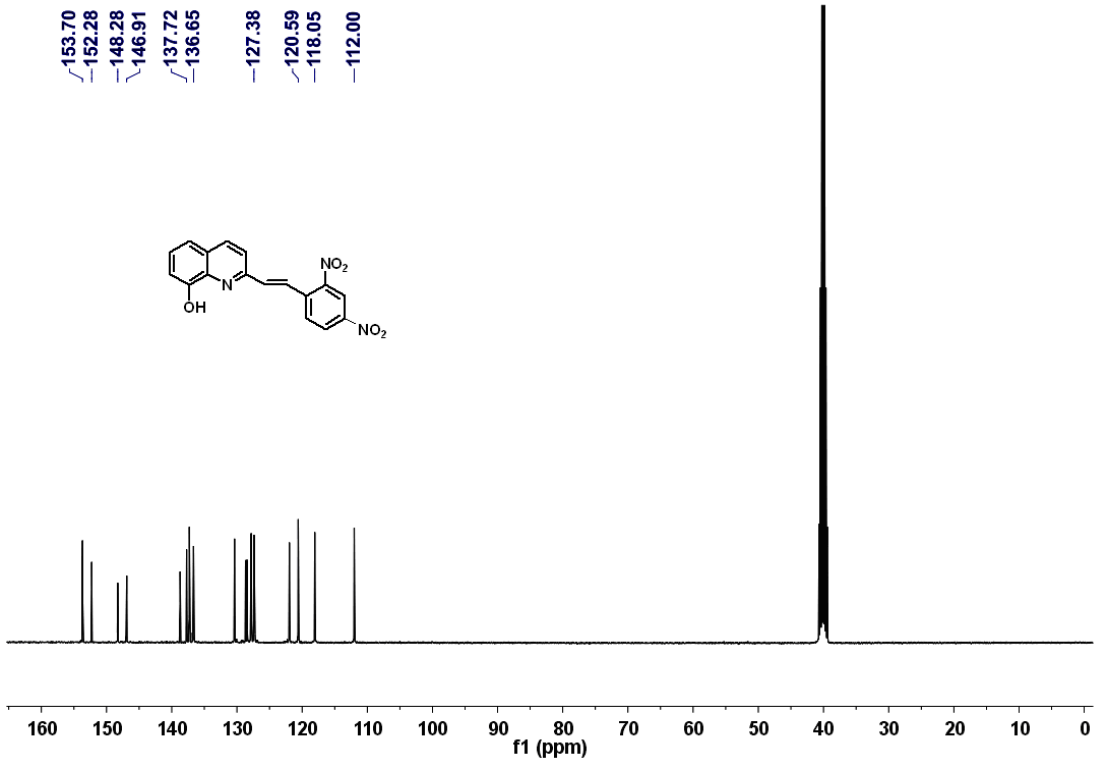


12. Figure S11. ^{1}H NMR, ^{13}C NMR spectra (d^6-DMSO) and ESI-MS of HL_2.

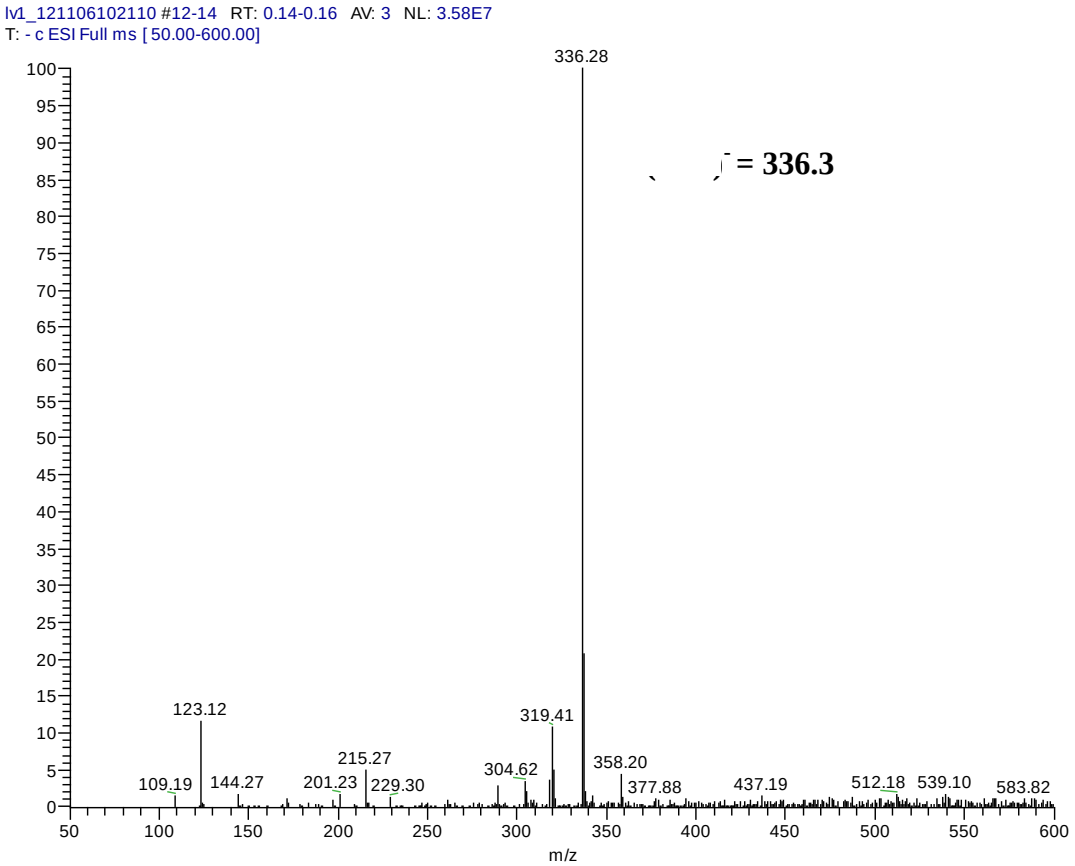
^{1}H NMR of HL_2



^{13}C NMR of HL_2

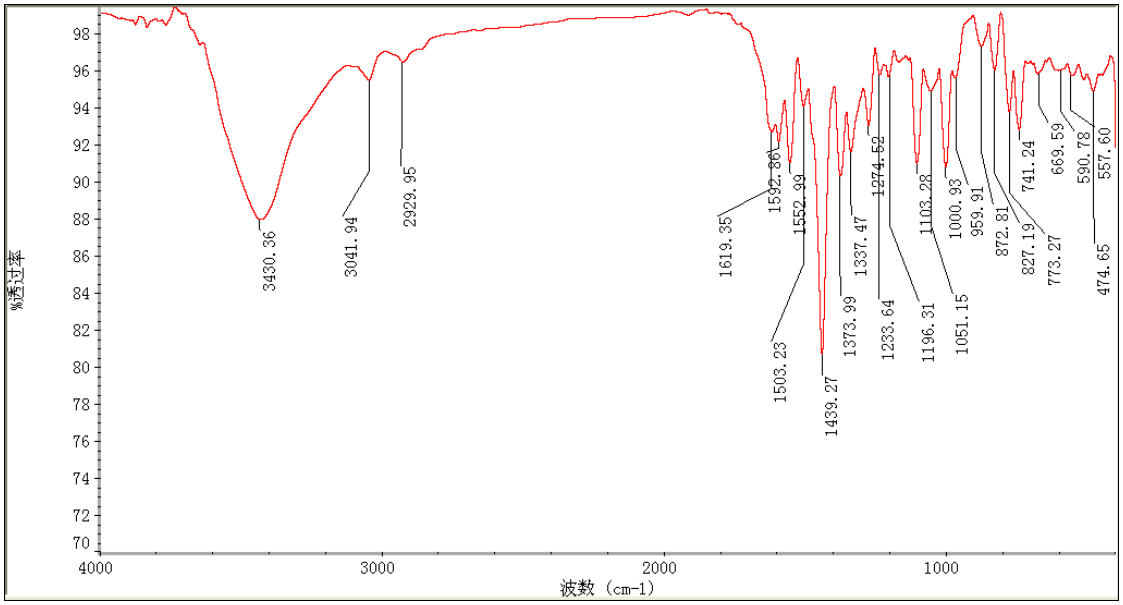


ESI-MS of HL_2



13. Figure S12. IR spectra of 1 and 2.

IR spectrum of 1



IR spectrum of 2