Supplementary Information

Synthesis, Characterization and computational studies of Zn complex based on 8-hydroxyquinoline group containing benzimidazole

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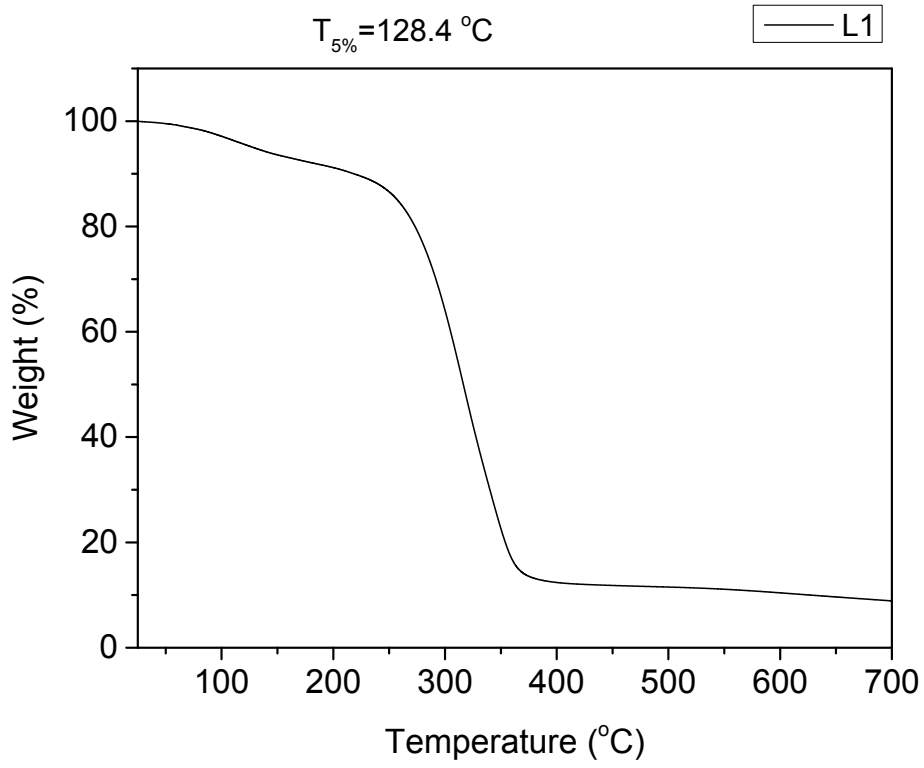

Fig. S1. TGA curves of compound L1 at a heating rate 20 K min^{-1}

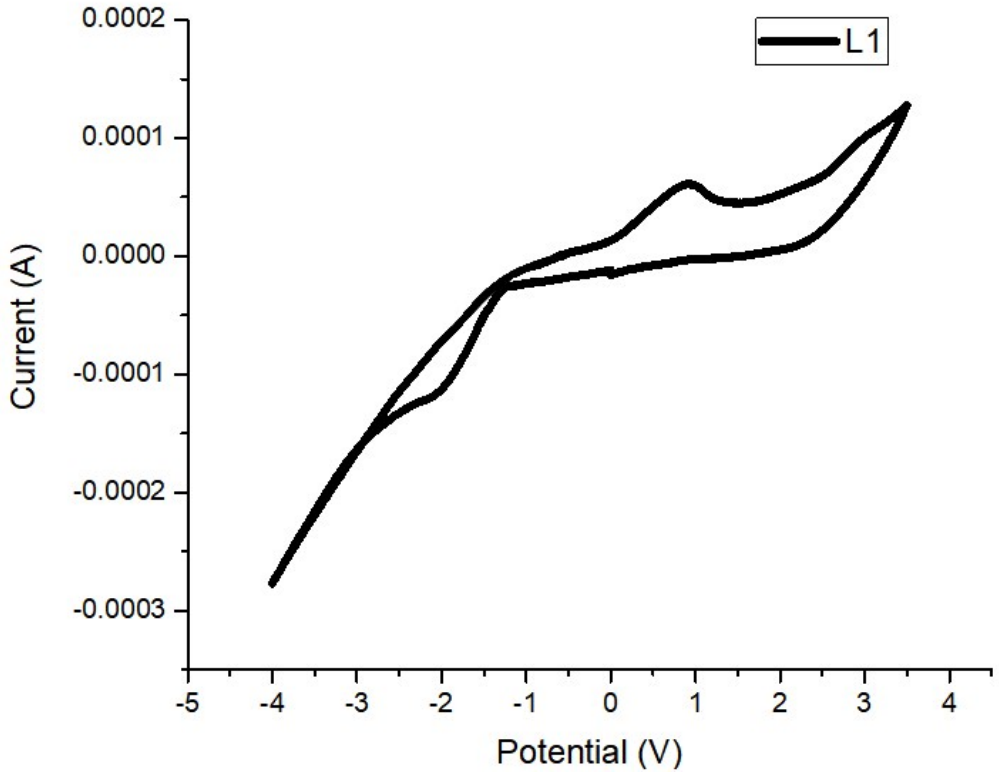

Fig. S2. Cyclic voltammograms of L1 in a solution of n-Bu_4NPF_6 (0.1 M) in DMSO

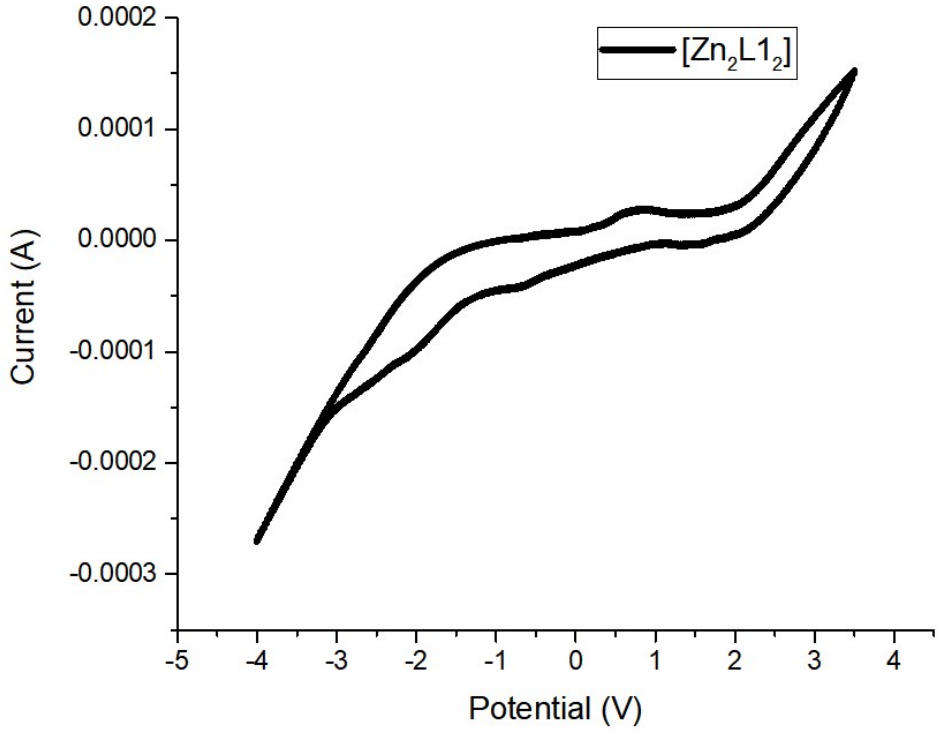

Fig. S3. Cyclic voltammograms of $[Zn_2L1_2]$ in a solution of n-Bu4NPF6 (0.1 M) in DMSO

Table S1. Crystal data and structure refinement for L1

Empirical formula	$C_{28}H_{24}N_4O_3$
Formula weight	464.51
Temperature/K	150.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.8401(2)
b/Å	15.7704(3)
c/Å	16.9216(5)

α/°	90.00
β/°	104.928(3)
γ/°	90.00
Volume/Å^3	2279.45(10)
Z	4
ρ_{calc}g/cm^3	1.354
μ/mm^{-1}	0.726
F(000)	976.0
Crystal size/mm^3	0.30 × 0.30 × 0.20
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.78 to 133.86
Index ranges	-10 ≤ h ≤ 6, -18 ≤ k ≤ 18, -19 ≤ l ≤ 20
Reflections collected	19470
Independent reflections	4047 [R_{int} = 0.0369, R_{sigma} = 0.0230]
Data/restraints/parameters	4047/0/350
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0431, wR_2 = 0.1188
Final R indexes [all data]	R_1 = 0.0537, wR_2 = 0.1309
Largest diff. peak/hole / e Å^{-3}	0.19/-0.23

Table S2. Selected bond distances (Å) and bond angles (o) with estimated standard deviations (e.s.d.s) in parentheses for L1

C1 - O1	1.360(2)	C21 - C22	1.417(2)

C4 - C5	1.414(3)	C22 - N4	1.370(2)		
C5 - C9	1.410(3)	C23 - O2	1.348(2)		
C6 - N1	1.361(2)	C24 - C25	1.389(3)		
C7 - N1	1.319(2)	O3 - C27	1.433(9)		
C10- N2	1.377(2)	C27 - H27D	0.9900		
C10- N3	1.322(2)	C27 - C28	1.469(9)		
C11- N3	1.387(2)	C28 - H28F	0.9800		
C12- N2	1.385(2)	O3' - C27'	1.358(14)		
C17- N2	1.468(2)	C28'- H28B	0.9800		
C18- N4	1.316(2)				

O1- C1- C2	121.26(16)	C26- C21- C22	119.61(16)		
O1- C1- C6	118.49(15)	C21- C22- C23	118.34(16)		
C1- C2- C3	120.24(18)	N4 - C22- C21	122.69(15)		
C4- C3- C2	121.31(17)	N4 - C22- C23	118.96(15)		
C6- C5- C4	118.97(17)	O2 - C23- C22	121.27(16)		
N1- C6- C5	123.57(15)	C7 - N1 - C6	117.82(14)		
C8- C7- C10	119.15(15)	C10- N2 - C12	106.20(13)		
N1- C7- C8	122.92(15)	C10- N2 - C17	130.66(13)		
N1- C7- C10	117.93(14)	C12- N2 - C17	123.09(14)		
C9- C8- C7	119.20(17)	C10- N3 - C11	105.13(14)		
C8- C9- C5	120.16(17)	C18- N4 - C22	118.11(14)		

Table S3. Crystal data and structure refinement for $[Zn_2L1_2]$

Empirical formula	$C_{52}H_{32}N_8O_4Zn_2$
Formula weight	963.60
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.4106(3)
b/Å	12.2137(3)
c/Å	20.5158(6)
α/°	87.203(2)
β/°	76.153(2)
γ/°	70.627(2)
Volume/Å^3	2617.48(12)
Z	2
ρ_{calc}g/cm^3	1.223
μ/mm^{-1}	1.519
F(000)	984.0
Crystal size/mm^3	0.3 × 0.2 × 0.15
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.68 to 150.28
Index ranges	$-9 \leq h \leq 14$, $-15 \leq k \leq 13$, $-25 \leq l \leq 24$
Reflections collected	21878
Independent reflections	10412 [R_{int} = 0.0628, R_{sigma} = 0.0759]
Data/restraints/parameters	10412/0/713
Goodness-of-fit on F^2	1.040

Final R indexes [I>=2σ (I)]	R_1 = 0.0673, wR_2 = 0.1809
Final R indexes [all data]	R_1 = 0.0841, wR_2 = 0.1992
Largest diff. peak/hole / e Å^{-3}	1.24/-0.92

Table S4. Selected bond distances (Å) and bond angles (o) with estimated standard deviations (e.s.d.s) in parentheses for [Zn_2L1_2]

Zn1-	O4	2.021(3)	O0AA-	C0FA	1.315(5)		
Zn1-	N5	2.186(3)	O2AA-	C8CA	1.304(5)		
Zn1-	N7CA	2.162(3)	O4 -	C8EA	1.318(5)		
Zn1-	N20	2.041(3)	O11 -	C0AA	1.321(5)		
Zn1-	O0AA	1.999(3)	O6 -	C5	1.410(9)		
Zn2-	O2AA	2.021(3)	N2 -	C7DA	1.458(5)		
Zn2-	O11	1.997(3)	N2 -	C8AA	1.357(5)		
Zn2-	N5CA	2.166(3)	N2 -	C9AA	1.388(5)		
Zn2-	N7	2.195(3)	N5 -	C0CA	1.325(5)		
Zn2-	N19	2.077(3)	N7 -	C3AA	1.361(5)		

O0AA-	Zn1	- N5	79.13(12)	N7	- C2AA-	C6CA	114.0(3)				
O4	- Zn1	- N20	95.32(12)	C0EA-	C2BA-	C7DA	116.8(3)				
N20	- Zn1	- N5	96.05(12)	C0FA-	O0AA-	Zn1	116.1(2)				
O2AA-	Zn2	- N7	167.61(12)	C8CA-	O2AA-	Zn2	114.0(2)				
O2AA-	Zn2	- N19	94.06(12)	C8EA-	O4	- Zn1	111.1(2)				
O11	- Zn2	- O2AA	89.47(11)	C0AA-	O11	- Zn2	116.5(2)				

O11 - Zn2 - N5CA	124.02(11)	C8AA- N2 - C7DA	125.3(3)
N19 - Zn2 - N5CA	112.97(12)	C4BA- N5 - Zn1	109.5(2)
N19 - Zn2 - N7	95.36(11)	C7BA- N5CA- Zn2	108.4(2)
N7CA- C0DA- C5DA	122.4(4)	C8EA- C8DA- C13	121.3(4)
N7CA- C0DA- C8EA	116.8(3)	O4 - C8EA - C0DA	118.3(3)
C5DA- C0DA- C8EA	120.8(4)	O4 - C8EA - C8DA	124.1(4)
C9EA - C0EA- C2BA	119.6(4)	C8DA- C8EA - C0DA	117.6(4)