SUPPLEMETARY MATERIALS

An efficient Vanillinyl Schiff base as a turn on fluorescent probe for Zinc(II) and Cell imaging

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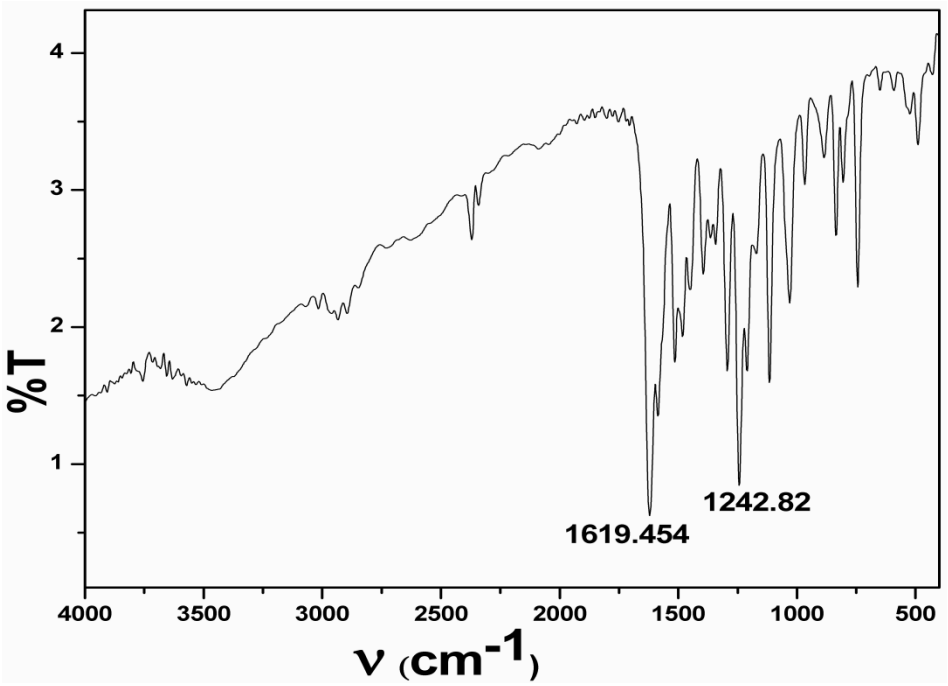

Fig. S1. FT-IR spectrum of H_2L in KBr disc

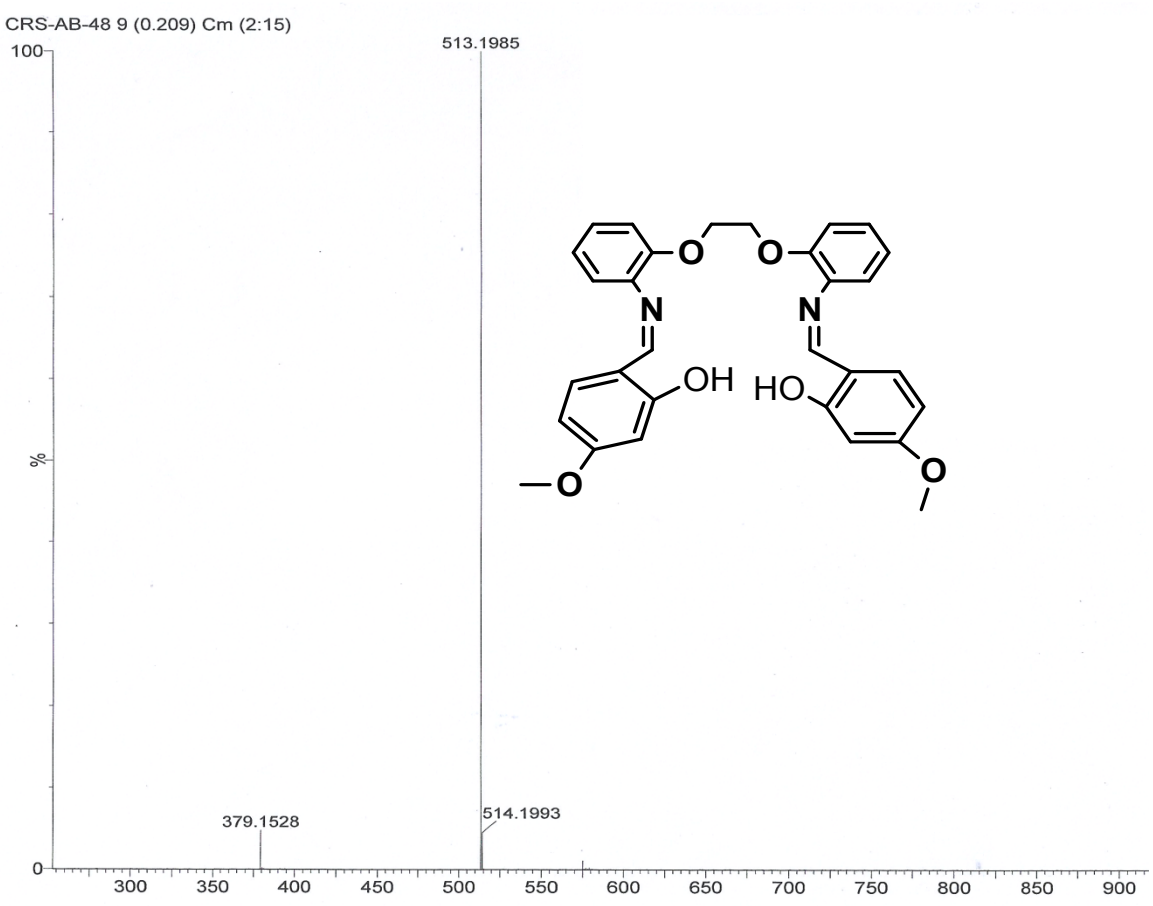

Fig. S2. Mass spectrum of H_2L

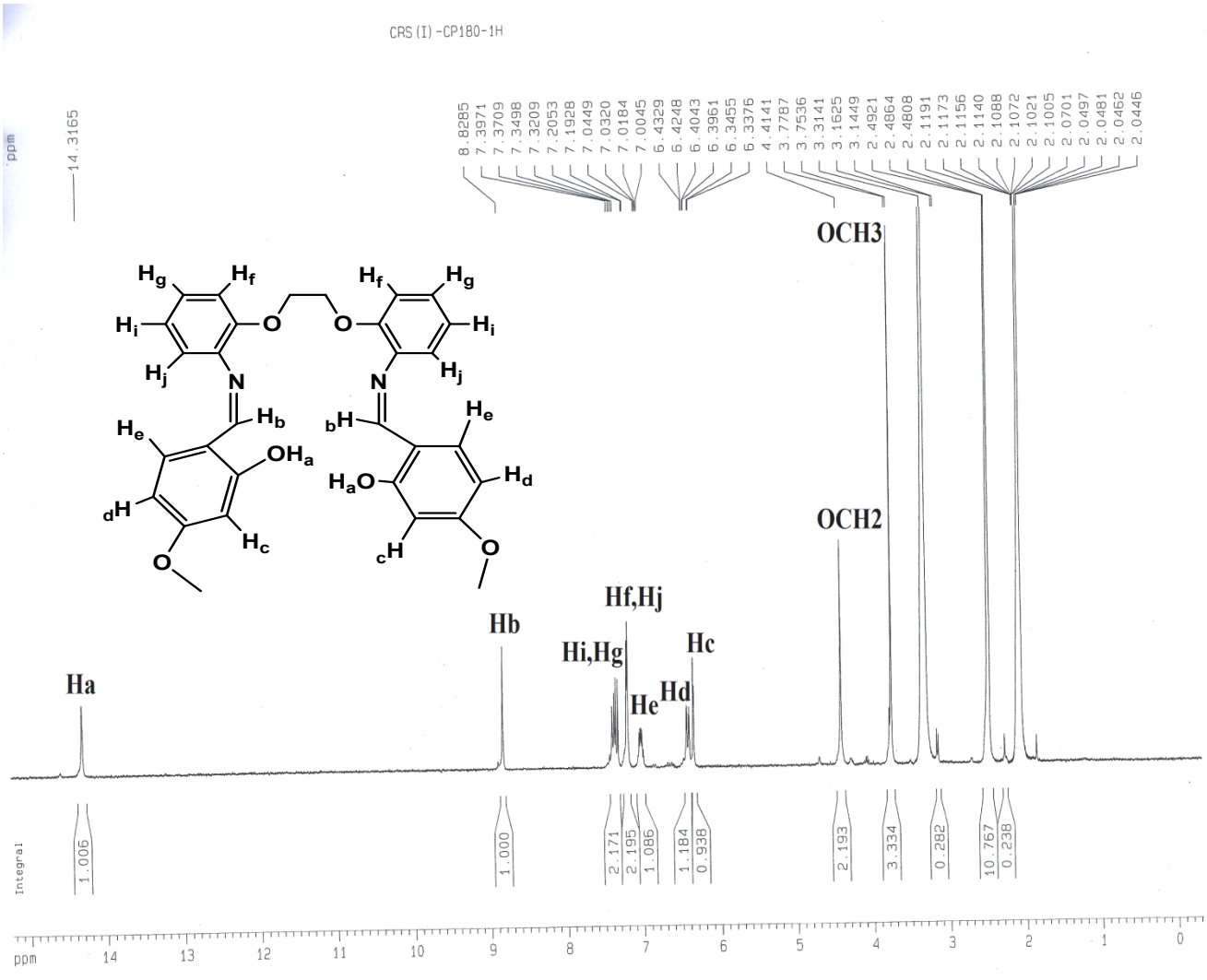

Fig. S3. ^{1}HNMR spectrum of H_2L in $CDCl_3$

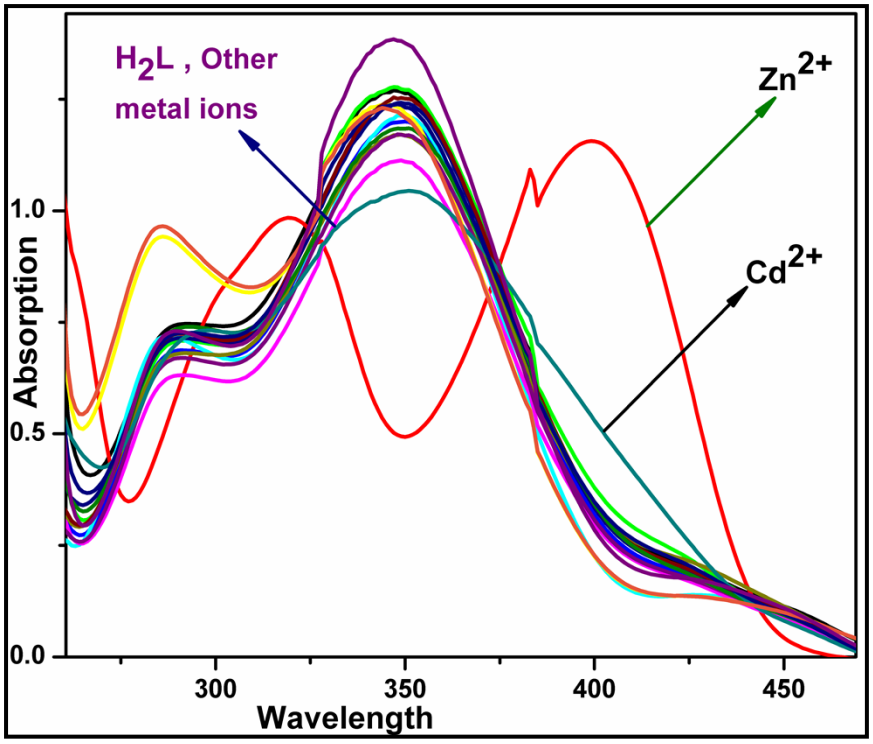

Fig: S4. Absorbance spectra of H_2L upon addition of various metal ions in DMSO– buffer (HEPES, pH = 7.4) (v/v = 3/7) solution

OPTICAL DETECTION LIMIT:

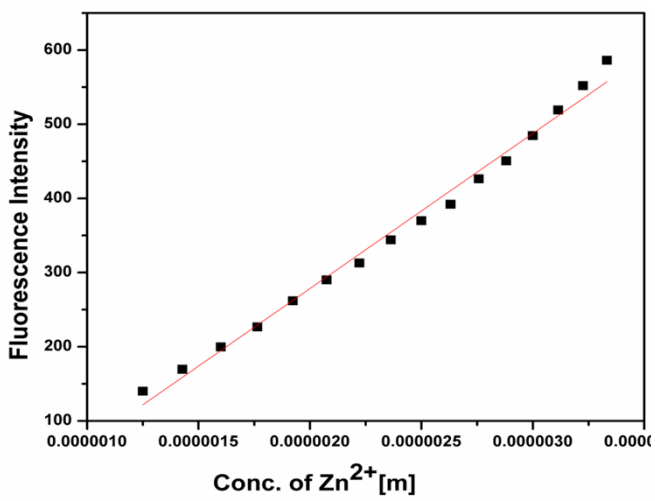

Fig. S4. The linear dynamic response of H_2L for Zn^{2+} and the determination of the detection limit (LOD) for Zn^{2+}

BINDING CONSTANT

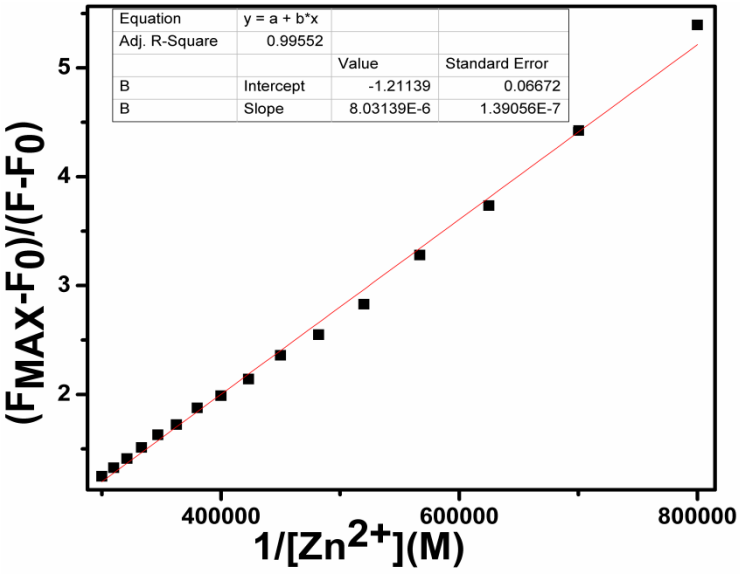

Fig. S5. Benesi-Hildebrand plot of {(*F*max-*F*o)/(*F*-*F*o)} vs. 1/[Zn2+].

Benesi-Hildebrand equation is given as: 

F_0 is the fluorescence of HL in the absence of externally added Zn^{2+} , F is the fluorescence obtainedat different [Zn^{2+}] (λex = 346 nm and λem = 470 nm] and with Fmax is the fluorescence of HL at [Zn^{2+}] in large excess. K (M-2) is the association constant.

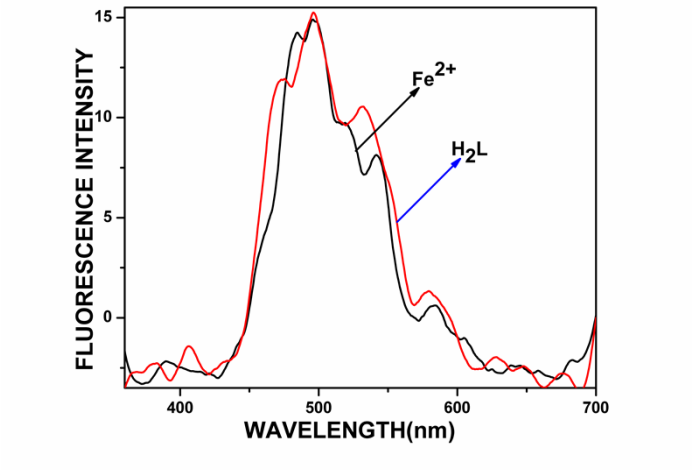

Fig. S6.. Change in fluorescence intensity of H_2L upon addition of 50 µM Fe^{2+} in DMSO/Water (HEPES buffer, pH, 7.4; v/v, 3/7).

Fig. S7. Comparison of emission of H_2L and [ZnL] under illumination in UV chamber

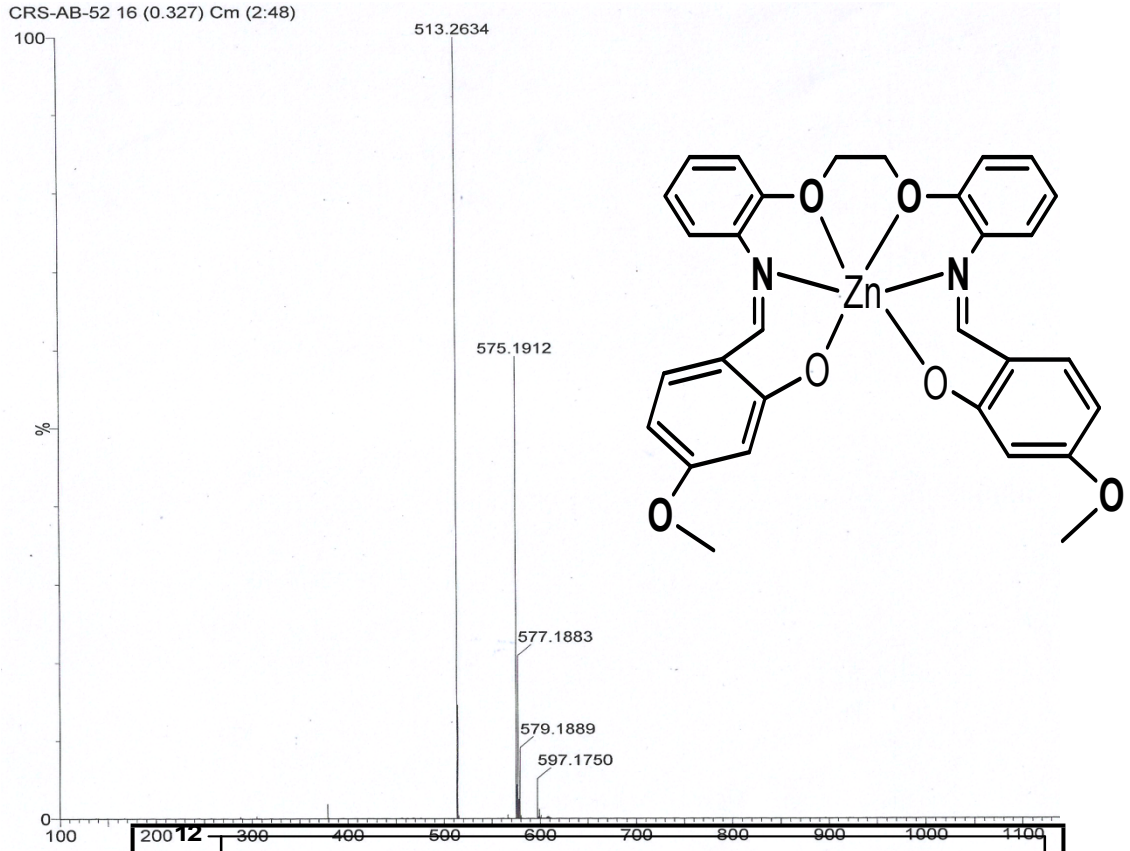

Fig. S8. Mass spectrum of [ZnL]

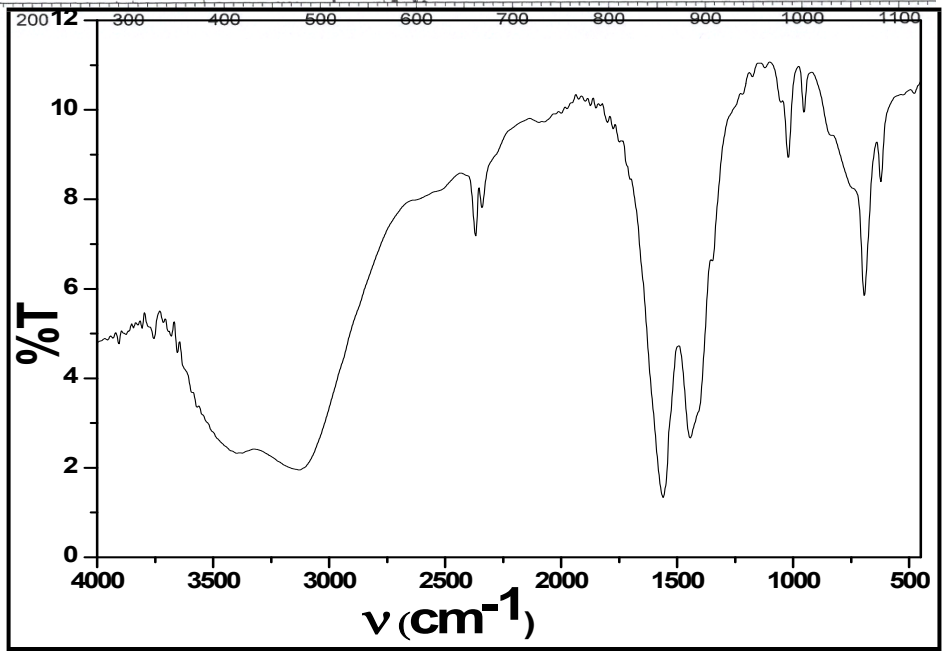

Fig. S9. FT-IR spectrum of [ZnL] in KBr disc

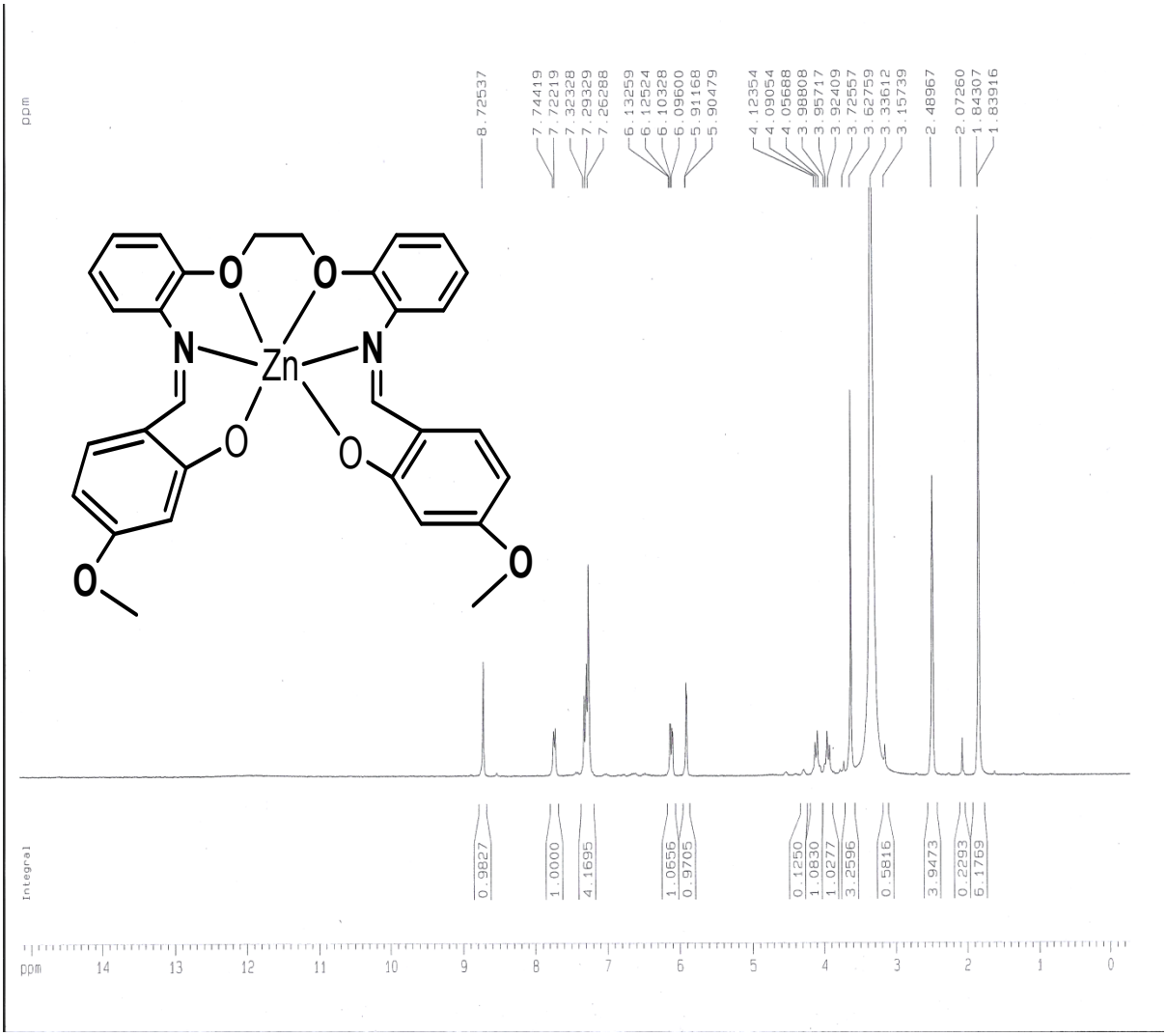

Fig. S10. ^{1}H NMR spectrum of [ZnL] in DMSO-d_6

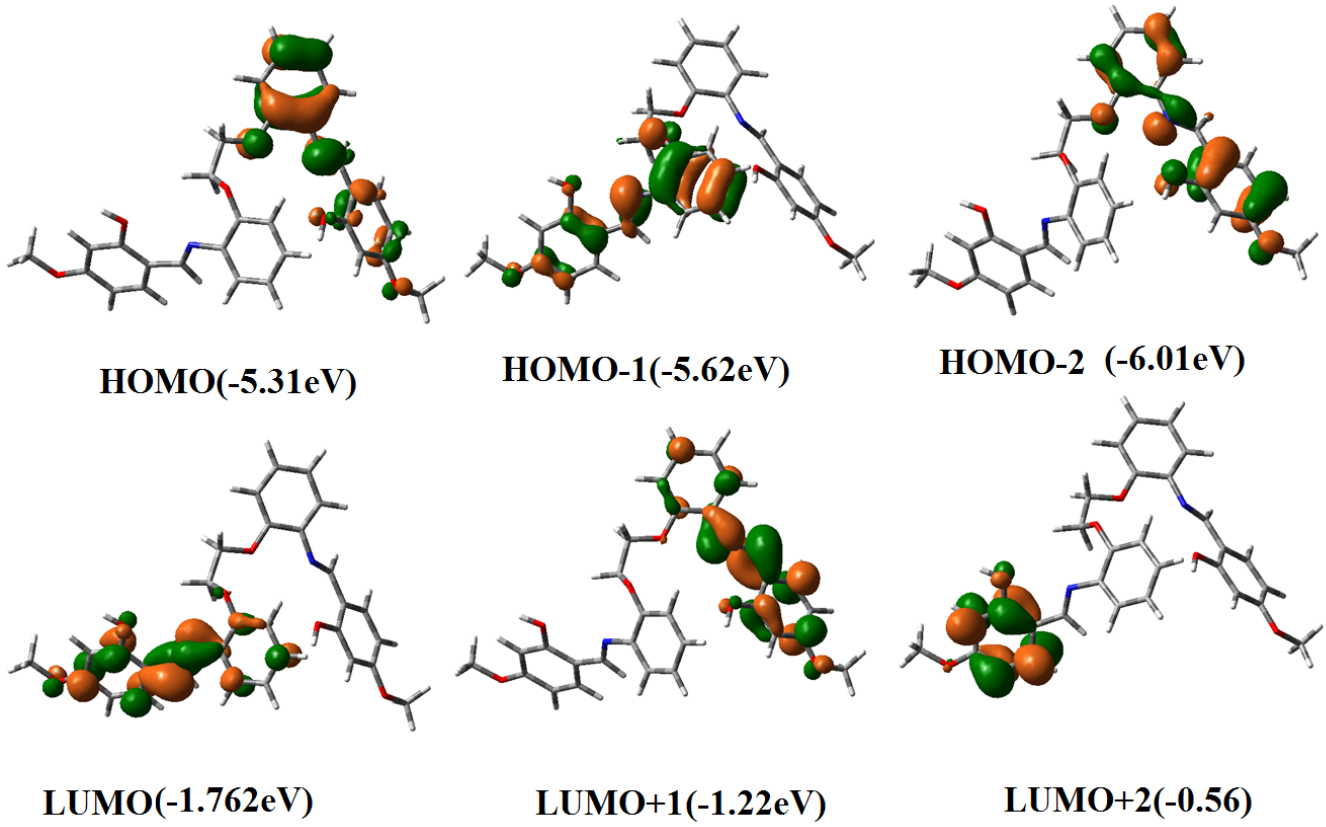

Fig S11: Frontier molecular orbitals of H_2L

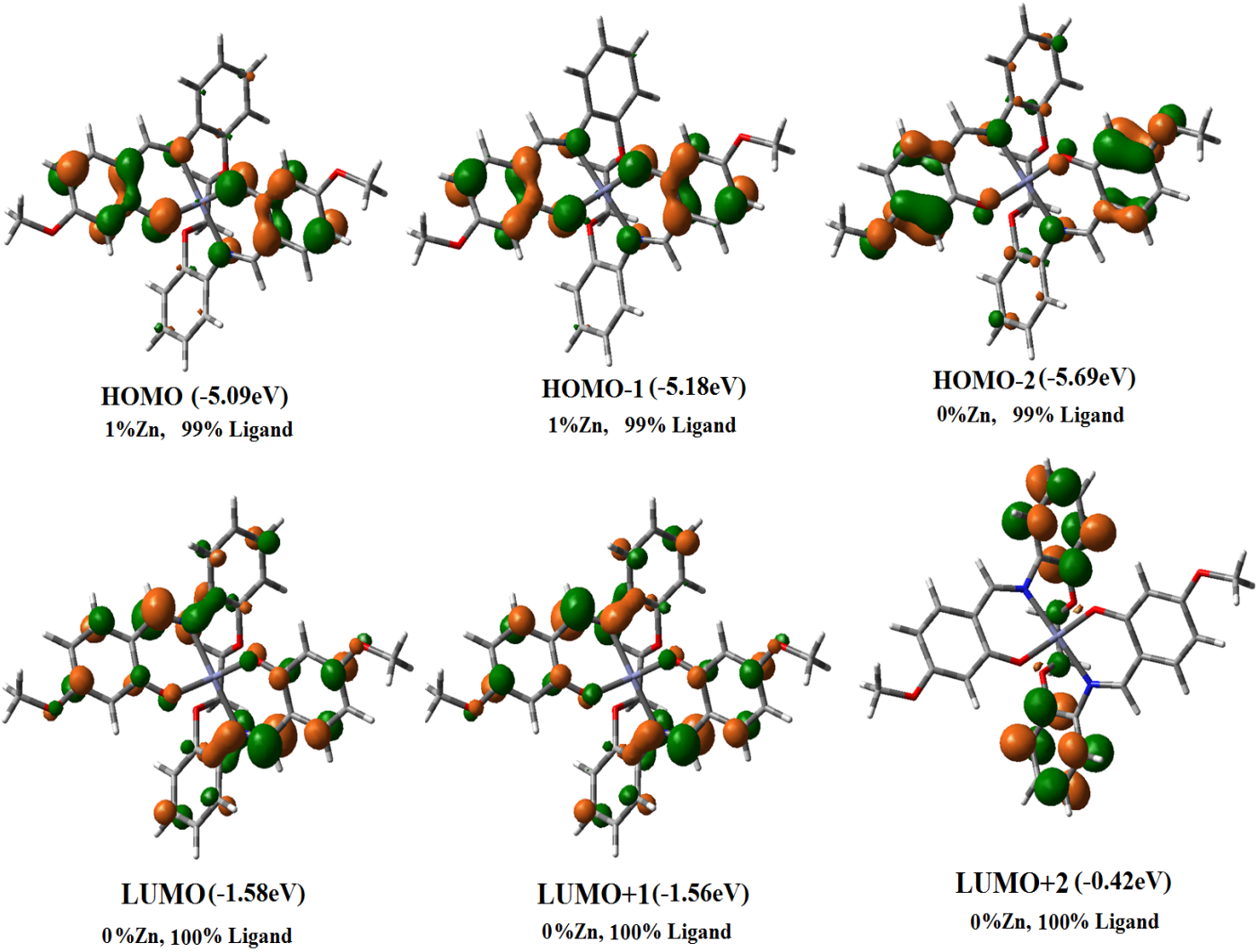

Fig S11: Frontier molecular orbitals of [ZnL]

Table S1. Composition and energy of MOs [ZnL]

Orbital	Energy(eV)	Composition	
		Metal	Ligand
LUMO+10	1.61	14	86
LUMO+9	1.56	3	97
LUMO+8	1.43	9	91
LUMO+7	0.54	1	99
LUMO+6	0.54	0	100
LUMO+5	0.14	1	99
LUMO+4	0.12	1	99
LUMO+3	-0.38	1	99
LUMO+2	-0.42	0	100
LUMO+1	-1.56	0	100
LUMO	-1.58	0	100
HOMO	-5.09	1	99
HOMO-1	-5.18	1	99
HOMO-2	-5.69	0	100
HOMO-3	-5.72	0	100
HOMO-4	-6.16	2	98
HOMO-5	-6.28	2	98
HOMO-6	-6.77	1	99
HOMO-7	-6.87	1	99
HOMO-8	-7.01	0	100
HOMO-9	-7.02	0	100
HOMO-10	-7.86	3	97

Table S2: Comparison of theoretical and experimental spectral transitions and their assignment in H_2L and [ZnL]

Compd	Experimental [λ_{exp}(nm)]	Theoretical [λ_{theo} (nm)]	Electronic Transition	f	Character
HL	373	362	$S_0 \rightarrow S_2$ [HOMO-1→ LUMO (86%)]	0.2995	ILCT
HL	290	303	$S_0 \rightarrow S_6$ [HOMO-3→ LUMO (72%),	0.1216	ILCT
[ZnL]	400	392	$S_0 \rightarrow S_1$ [HOMO→LUMO(98%)]	0.1013	ILCT
[ZnL]	316	331	$S_0 \rightarrow S_4$ [HOMO-2→LUMO (82%)]	0.4958	ILCT

Table S3: Bond parameters of H_2L

Bond Distance (Å)		Bond angle (°)	
O(1)-C(2) C(17)-O(18)	1.353 1.361	O(1)-C(2)-C(3)	118.35
C(4)-N(5) N(14)-C(15)	1.281 1.283	C(4)-N(5)-C(6)	120.59
N(5)-C(6) C(13)-N(14)	1.398 1.404	C(7)-O(8)-C(9)	119.98
C(7)-O(8) O(11)-C(12)	1.361 1.366	C(9)-C(10)-O(11)	108.36
O(8)-C(9) C(10)-O(11)	1.421 1.434	C(10)-O(11)-C(12)	121.20

Table S4: Bond parameters of [ZnL]

Bond Distance (Å)		Bond angle (°)	
Zn-O(1) Zn-O(18)	1.993 1.993	O(1)-Zn-N(5) O(18)-Zn-N(14)	88.66 88.66
Zn-N(5) Zn-N(14)	2.131 2.132	N(5)-Zn-O(8) N(14)-Zn-O(11)	71.17 71.16
Zn-O(8) Zn-O(8)	2.493 2.492	O(8)-Zn-O(18) O(11)-Zn-O(1)	88.66 88.67
O(1)-C(2) C(17)-O(18)	1.317 1.317	O(1)-C(2)-C(3)	122.89
C(4)-N(5) N(14)-C(15)	1.325 1.326	C(4)-N(5)-C(6)	120.65
C(7)-O(8) O(11)-C(12)	1.419 1.420	C(7)-O(8)-C(9)	114.95
O(8)-C(9) C(10)-O(11)	1.474 1.475	C(9)-C(10)-O(11)	106.59