Electronic Supplementary Information

Naphthalene-thiophene hybrid molecule as a fluorescent AND logic gate with Zn^{2+} and OAc^{-} ions as inputs: Cell imaging and computational studies

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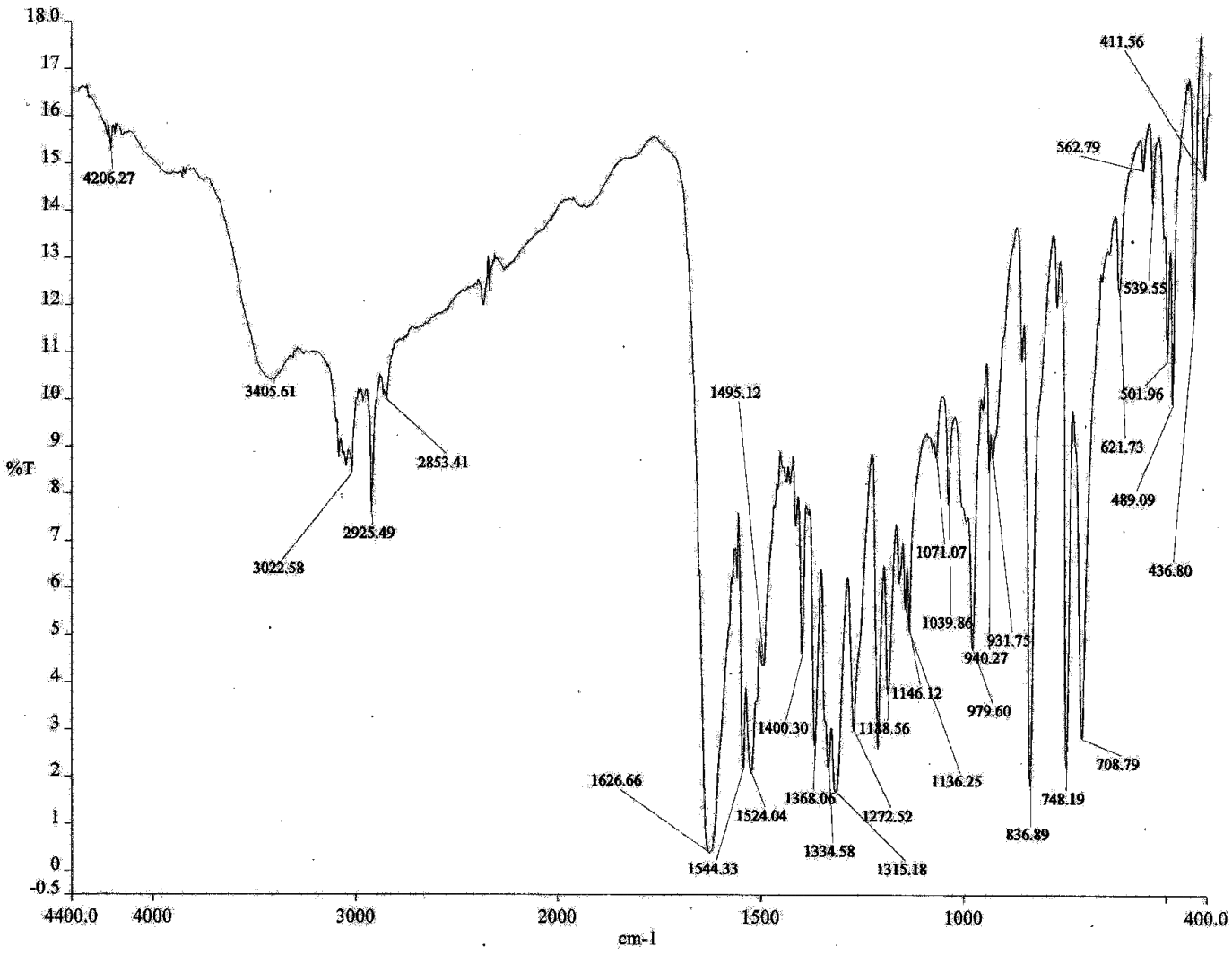

Fig. S1 FTIR spectrum of **HL**.

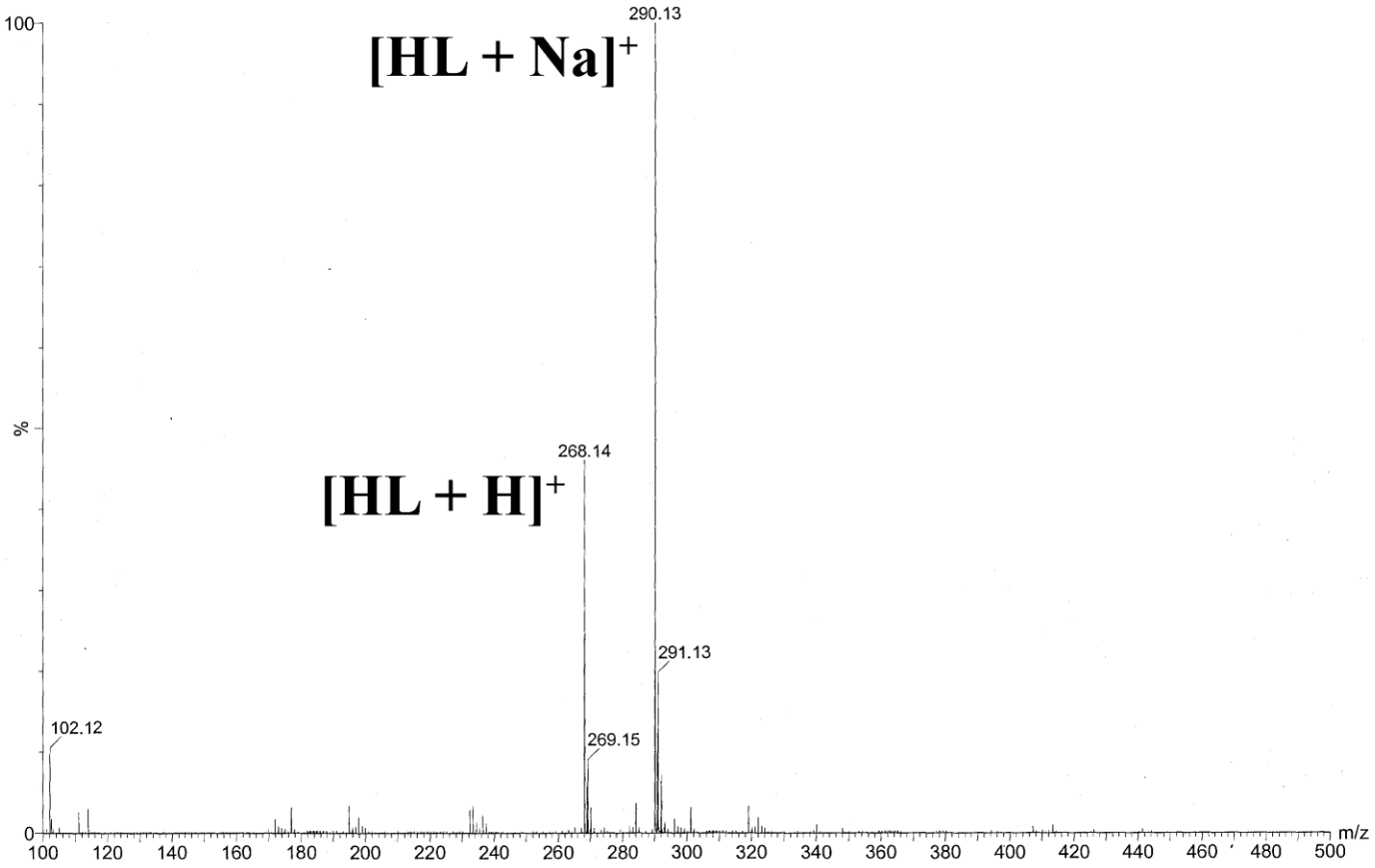

Fig. S2 QTOF-MS$^+$ spectrum of **HL**.

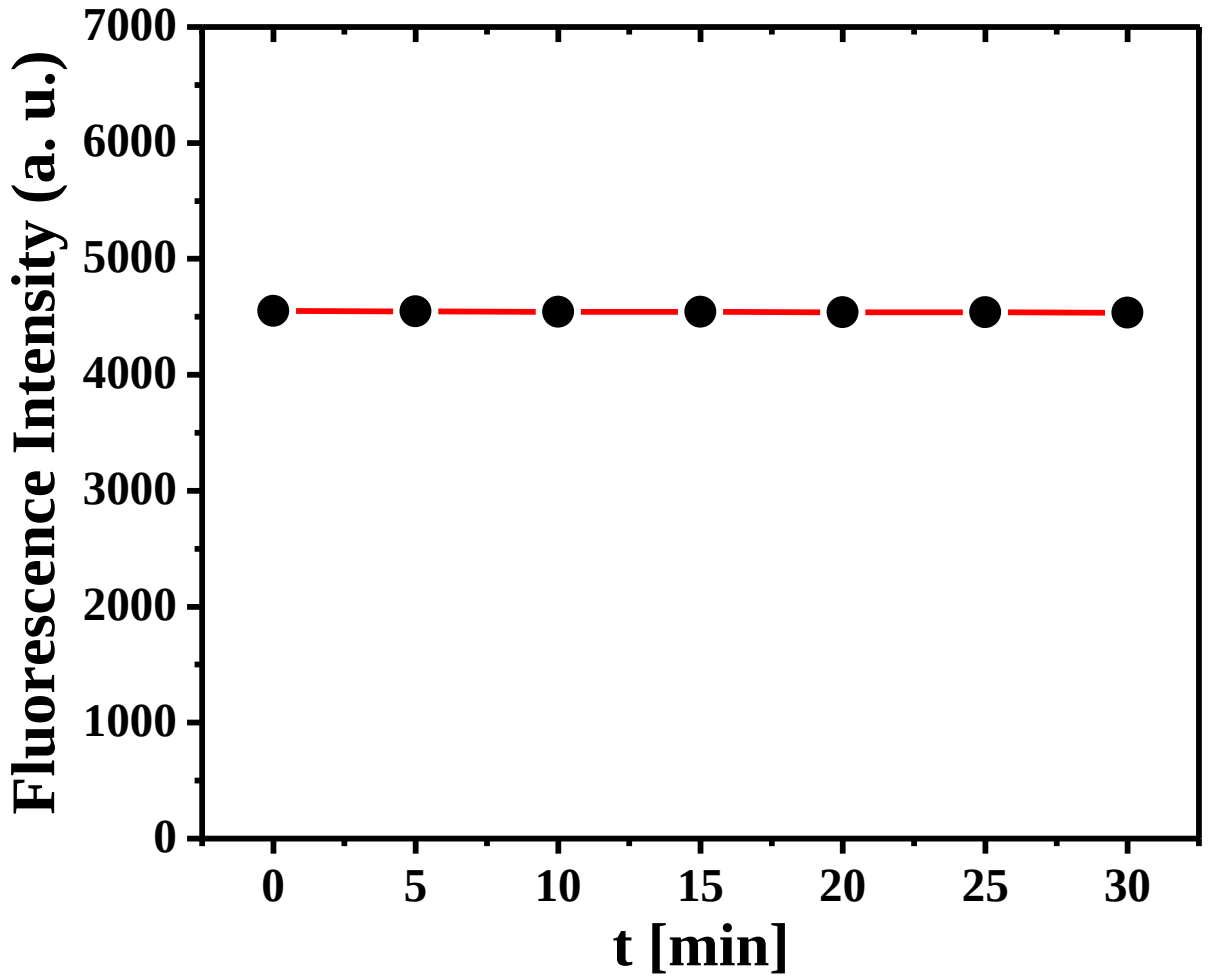

Fig. S3 Variation of the emission intensity of the [**L**–$Zn(OAc)_2$] system with time.

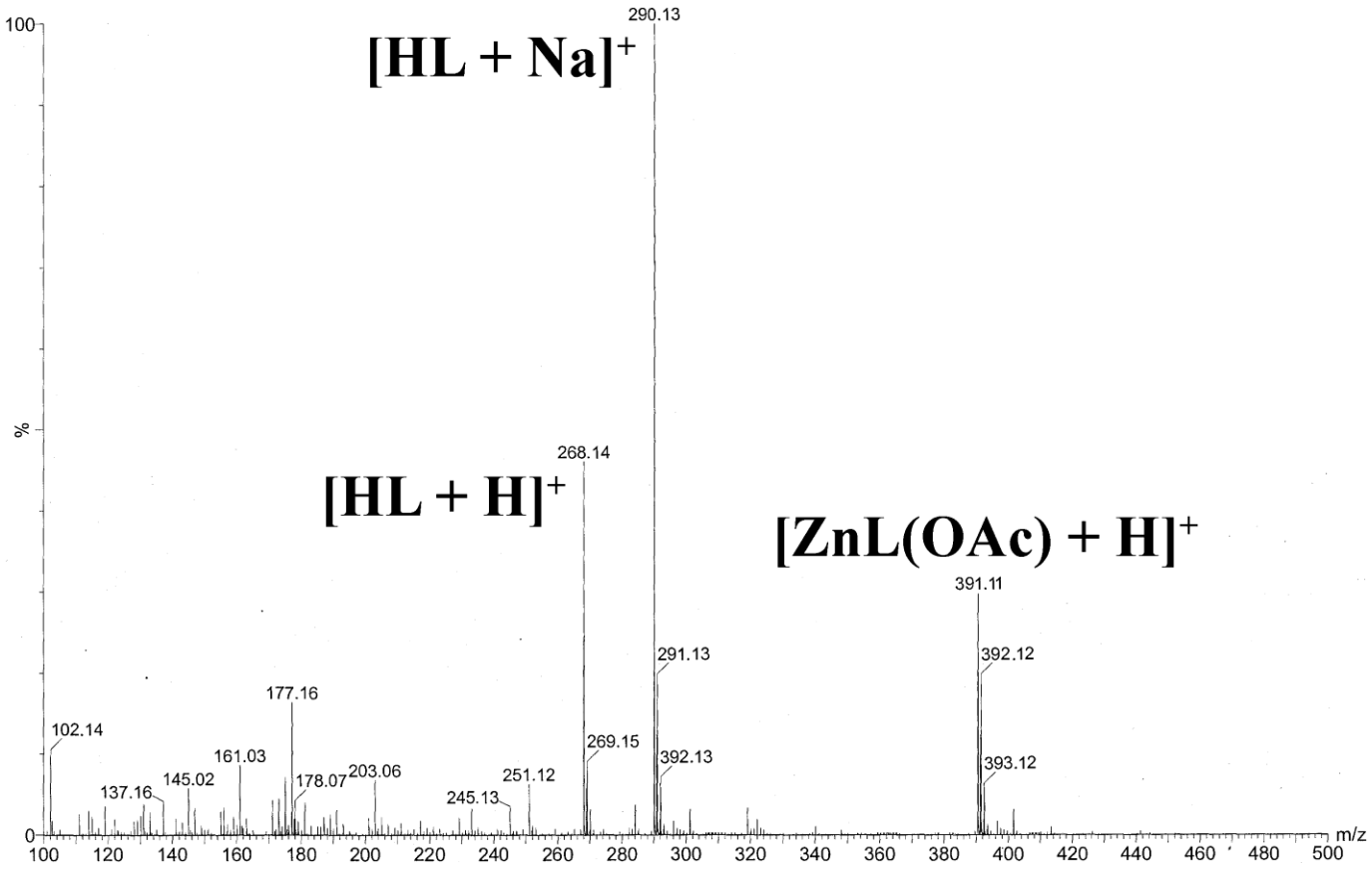

Fig. S4 QTOF-MS$^+$ spectrum of the **[ZnL(OAc)]** complex.

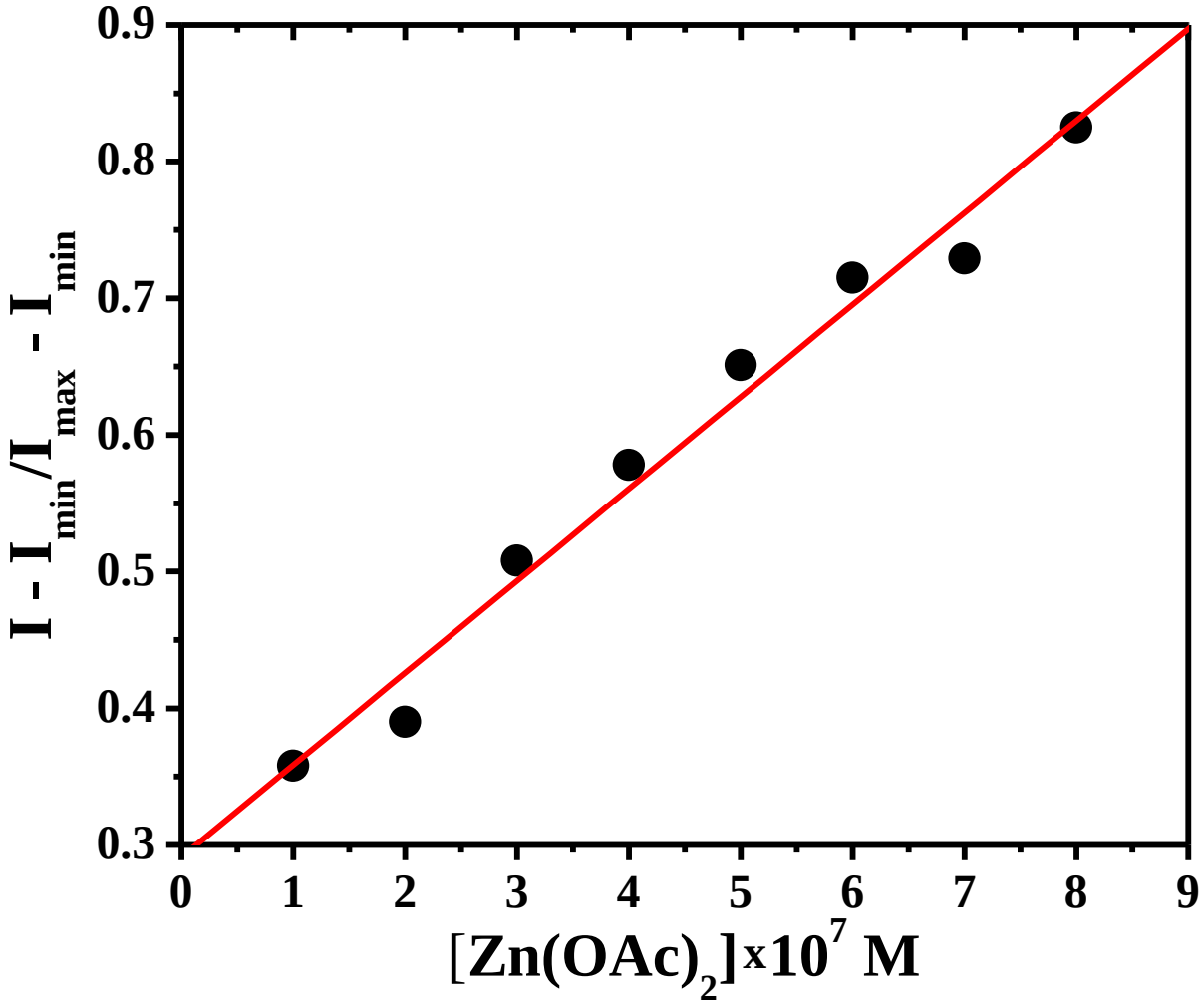

Fig. S6 Determination of the detection limit of $Zn(OAc)_2$ by **HL** (0.1 μM, EtOH–H_2O (1:1, v/v), 0.1 M HEPES buffer, pH 7.4, λ_{em} = 448 nm). Emission intensity of **HL** is plotted as a function of $Zn(OAc)_2$ (1, 2, 3, 4, 5, 6, 7, 8, 9 and 10 μM), normalized between the minimum and maximum emission intensities. The point at which the best fitted line crosses the abscissa by extrapolation is LOD.

Table S1 Selected bond lengths (Å) and bond angles (°) for **HL**

Bond lengths					
O(1)–C(12)	1.264(3)	C(12)–C(13)	1.447(3)	C(18)–C(19)	1.369(4)
N(1)–C(1)	1.308(3)	C(13)–C(14)	1.345(4)	C(19)–C(20)	1.405(3)
N(1)–C(2)	1.470(3)	C(14)–C(15)	1.425(4)	C(21)–C(25)	1.606(3)
C(1)–C(11)	1.402(3)	C(15)–C(16)	1.409(3)	C(21)–S(22)	1.615(3)
C(2)–C(21)	1.502(3)	C(15)–C(20)	1.417(3)	S(22)–C(23)	1.544(4)
C(11)–C(12)	1.436(3)	C(16)–C(17)	1.360(4)	C(23)–C(24)	1.320(6)
C(11)–C(20)	1.456(3)	C(17)–C(18)	1.399(4)	C(24)–C(25)	1.535(4)
Bond angles					
C(1)–N(1)–C(2)	123.5(2)	C(13)–C(14)–C(15)	122.7(2)	C(19)–C(20)–C(11)	123.92(19)
N(1)–C(1)–C(11)	124.9(2)	C(16)–C(15)–C(20)	120.0(2)	C(15)–C(20)–C(11)	118.9(2)
N(1)–C(2)–C(21)	113.77(19)	C(16)–C(15)–C(14)	121.0(2)	C(2)–C(21)–C(25)	124.1(2)
C(1)–C(11)–C(12)	118.9(2)	C(20)–C(15)–C(14)	119.0(2)	C(2)–C(21)–S(22)	124.1(2)
C(1)–C(11)–C(20)	120.5(2)	C(17)–C(16)–C(15)	121.4(2)	C(25)–C(21)–S(22)	111.76(16)
C(12)–C(11)–C(20)	120.60(19)	C(16)–C(17)–C(18)	118.7(2)	C(23)–S(22)–C(21)	97.96(18)
O(1)–C(12)–C(11)	122.9(2)	C(19)–C(18)–C(17)	121.4(2)	C(24)–C(23)–S(22)	115.8(3)
O(1)–C(12)–C(13)	119.8(2)	C(18)–C(19)–C(20)	121.3(2)	C(23)–C(24)–C(25)	116.0(3)
C(11)–C(12)–C(13)	117.2(2)	C(19)–C(20)–C(15)	117.2(2)	C(24)–C(25)–C(21)	98.44(19)
C(14)–C(13)–C(12)	121.6(2)				

Table S2 Selected bond lengths (Å) and bond angles (°) for **$[H_3L_2]ClO_4$**

Bond lengths					
S(1)–C(16)	1.704(2)	C(10)–C(11)	1.406(3)	C(4A)–C(5A)	1.412(3)
S(1)–C(13)	1.714(2)	C(12)–C(13)	1.492(3)	C(5A)–C(6A)	1.366(3)
O(1)–C(1)	1.302(2)	C(13)–C(14)	1.389(3)	C(6A)–C(7A)	1.392(4)
N(1)–C(11)	1.298(2)	C(14)–C(15)	1.448(3)	C(7A)–C(8A)	1.371(3)
N(1)–C(12)	1.470(2)	C(15)–C(16)	1.345(3)	C(8A)–C(9A)	1.420(3)
C(1)–C(10)	1.420(2)	S(1A)–C(16A)	1.660(3)	C(9A)–C(10A)	1.457(3)
C(1)–C(2)	1.429(3)	S(1A)–C(13A)	1.720(2)	C(10A)–C(11A)	1.416(3)
C(2)–C(3)	1.348(3)	O(1A)–C(1A)	1.311(2)	C(12A)–C(13A)	1.496(3)
C(3)–C(4)	1.430(3)	N(1A)–C(11A)	1.291(3)	C(13A)–C(14A)	1.533(3)
C(4)–C(5)	1.407(3)	N(1A)–C(12A)	1.464(3)	C(14A)–C(15A)	1.480(3)
C(4)–C(9)	1.417(3)	C(1A)–C(10A)	1.417(3)	C(15A)–C(16A)	1.339(4)
C(5)–C(6)	1.368(3)	C(1A)–C(2A)	1.421(3)	Cl(1)–O(13)	1.404(2)
C(6)–C(7)	1.397(3)	C(2A)–C(3A)	1.351(3)	Cl(1)–O(11)	1.4141(18)
C(7)–C(8)	1.373(3)	C(3A)–C(4A)	1.426(3)	Cl(1)–O(12)	1.4260(16)
C(8)–C(9)	1.410(3)	C(4A)–C(9A)	1.410(3)	Cl(1)–O(14)	1.4372(19)
C(9)–C(10)	1.449(3)				
Bond angles					
C(16)–S(1)–C(13)	91.99(10)	N(1)–C(12)–C(13)	110.98(16)	C(4A)–C(9A)–C(8A)	117.36(19)
C(11)–N(1)–C(12)	123.98(17)	C(14)–C(13)–C(12)	126.83(19)	C(4A)–C(9A)–C(10A)	119.07(17)
O(1)–C(1)–C(10)	120.38(16)	C(14)–C(13)–S(1)	112.67(14)	C(8A)–C(9A)–C(10A)	123.57(19)
O(1)–C(1)–C(2)	120.76(16)	C(12)–C(13)–S(1)	120.49(16)	C(11A)–C(10A)–C(1A)	120.63(17)
C(10)–C(1)–C(2)	118.86(16)	C(13)–C(14)–C(15)	109.23(17)	C(11A)–C(10A)–C(9A)	119.61(17)
C(3)–C(2)–C(1)	120.60(17)	C(16)–C(15)–C(14)	114.19(18)	C(1A)–C(10A)–C(9A)	119.63(17)
C(2)–C(3)–C(4)	122.72(17)	C(15)–C(16)–S(1)	111.92(15)	N(1A)–C(11A)–C(10A)	127.09(18)
C(5)–C(4)–C(9)	120.17(17)	C(16A)–S(1A)–C(13A)	92.12(12)	N(1A)–C(12A)–C(13A)	111.15(16)
C(5)–C(4)–C(3)	121.22(17)	C(11A)–N(1A)–C(12A)	123.96(18)	C(12A)–C(13A)–C(14A)	124.28(18)
C(9)–C(4)–C(3)	118.60(17)	O(1A)–C(1A)–C(10A)	119.62(17)	C(12A)–C(13A)–S(1A)	121.92(16)
C(6)–C(5)–C(4)	121.04(18)	O(1A)–C(1A)–C(2A)	121.11(16)	C(14A)–C(13A)–S(1A)	113.75(15)
C(5)–C(6)–C(7)	119.06(18)	C(10A)–C(1A)–C(2A)	119.27(17)	C(15A)–C(14A)–C(13A)	101.79(17)
C(8)–C(7)–C(6)	121.12(19)	C(3A)–C(2A)–C(1A)	120.73(18)	C(16A)–C(15A)–C(14A)	117.6(2)
C(7)–C(8)–C(9)	121.22(18)	C(2A)–C(3A)–C(4A)	122.47(19)	C(15A)–C(16A)–S(1A)	114.7(2)
C(8)–C(9)–C(4)	117.27(17)	C(9A)–C(4A)–C(5A)	120.22(19)	O(13)–Cl(1)–O(11)	112.01(18)
C(8)–C(9)–C(10)	123.86(16)	C(9A)–C(4A)–C(3A)	118.80(18)	O(13)–Cl(1)–O(12)	109.30(14)
C(4)–C(9)–C(10)	118.87(16)	C(5A)–C(4A)–C(3A)	121.0(2)	O(11)–Cl(1)–O(12)	109.98(12)
C(11)–C(10)–C(1)	119.96(16)	C(6A)–C(5A)–C(4A)	120.9(2)	O(13)–Cl(1)–O(14)	108.27(19)
C(11)–C(10)–C(9)	119.81(16)	C(5A)–C(6A)–C(7A)	119.3(2)	O(11)–Cl(1)–O(14)	108.85(13)
C(1)–C(10)–C(9)	120.21(16)	C(8A)–C(7A)–C(6A)	121.3(2)	O(12)–Cl(1)–O(14)	108.34(12)
N(1)–C(11)–C(10)	125.48(17)	C(7A)–C(8A)–C(9A)	120.9(2)		

Table S3. Hydrogen bond lengths (Å) and angles (°) for **HL** and **$[H_3L_2]ClO_4$**

	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
HL	N(1)–H(1)···O(1)	0.92(4)	1.84(4)	2.596(3)	139(3)
$[H_3L_2]ClO_4$	N(1)–H(1)···O(1)	0.81(3)	1.93(3)	2.579(2)	137(2)
	N(1A)–H(1A)···O(1A)	0.82(3)	2.02(3)	2.630(2)	131(2)
	O(1A)–H(1O)···O(1)	1.17(4)	1.29(4)	2.4511(17)	179(3)

Table S4. Relevant bond lengths (Å) and angles (°) for **[ZnL(OAc)]**, obtained using the 6-31G basis set (atom numbering refers to Fig. 14)

Bond lengths					
Zn(15)–N(3)	1.95	Zn(15)–O(18)	2.06	C(1)–N(3)	1.32
Zn(15)–O(39)	1.89	Zn(15)–O(17)	2.10	O(39)–C(25)	1.32
Bond angles					
O(39)–Zn(15)–O(18)	123.74	O(39)–Zn(15)–N(3)	96.50	O(17)–Zn(15)–O(18)	64.48
N(3)–Zn(15)–O(18)	128.73	N(3)–Zn(15)–O(17)	117.20	O(39)–Zn(15)–O(17)	127.31

Table S5. Summary of the Natural Population Analysis (NPA) for **HL**

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	–0.22610	1.99900	4.21557	0.01153	6.22610
C	2	–0.23748	1.99898	4.22865	0.00986	6.23748
C	3	–0.01145	1.99894	4.00208	0.01042	6.01145
C	4	–0.08235	1.99891	4.07235	0.01109	6.08235
C	5	–0.20491	1.99897	4.19528	0.01066	6.20491
C	6	–0.25496	1.99899	4.2443	0.01168	6.25496
H	7	0.24382	0.00000	0.75515	0.00102	0.75618
H	8	0.22863	0.00000	0.77010	0.00127	0.77137
C	9	–0.21602	1.99891	4.20481	0.0123	6.21602
C	10	–0.17795	1.99897	4.16876	0.01022	6.17795
H	11	0.24102	0.00000	0.75770	0.00129	0.75898
H	12	0.24476	0.00000	0.75426	0.00098	0.75524
C	13	–0.28065	1.99893	4.26852	0.0132	6.28065
C	14	0.42623	1.99895	3.54884	0.02598	5.57377
H	15	0.24394	0.00000	0.75471	0.00134	0.75606
H	16	0.25697	0.00000	0.74121	0.00182	0.74303
O	17	–0.65548	1.99979	6.65195	0.00374	8.65548
C	18	0.11902	1.99908	3.86724	0.01465	5.88098
H	19	0.22797	0.00000	0.77068	0.00136	0.77203
N	20	–0.56068	1.99922	5.55152	0.00994	7.56068
C	21	–0.29988	1.99904	4.28795	0.01289	6.29988
H	22	0.25426	0.00000	0.74368	0.00206	0.74574
H	23	0.26791	0.00000	0.72998	0.00211	0.73209
C	24	–0.19492	1.99885	4.18080	0.01527	6.19492
C	25	–0.28455	1.99875	4.27428	0.01153	6.28455
S	26	0.34053	9.99934	5.64639	0.01374	15.65947
C	27	–0.27975	1.99888	4.26883	0.01204	6.27975
H	28	0.26870	0.00000	0.72964	0.00166	0.73130
C	29	–0.39437	1.99894	4.38343	0.01200	6.39437
H	30	0.25952	0.00000	0.73972	0.00076	0.74048
H	31	0.26528	0.00000	0.73404	0.00067	0.73472
H	32	0.47294	0.00000	0.52145	0.00561	0.52706
Total		0.00000	45.98144	93.76387	0.25469	140.00000

Table S6. Summary of the Natural Population Analysis (NPA) for **[ZnL(OAc)]**

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.13199	1.99916	3.84887	0.01999	5.86801
H	2	0.21075	0.00000	0.78707	0.00218	0.78925
N	3	–0.72784	1.99938	5.70013	0.02833	7.72784
C	4	–0.31512	1.99901	4.29810	0.01801	6.31512
H	5	0.24847	0.00000	0.74929	0.00224	0.75153
H	6	0.27382	0.00000	0.72361	0.00258	0.72618
C	7	–0.20233	1.99882	4.18747	0.01603	6.20233
C	8	–0.27952	1.99875	4.26910	0.01166	6.27952
S	9	0.37377	9.99932	5.61105	0.01586	15.62623
C	10	–0.28713	1.99888	4.27613	0.01211	6.28713
H	11	0.25245	0.00000	0.74664	0.00091	0.74755
C	12	–0.39507	1.99895	4.38381	0.01232	6.39507
H	13	0.25756	0.00000	0.74167	0.00078	0.74244
H	14	0.26622	0.00000	0.73309	0.00069	0.73378
Zn	15	1.58550	17.99821	10.34388	0.07241	28.4145
C	16	0.75458	1.99942	3.19315	0.05285	5.24542
O	17	–0.77000	1.99980	6.76505	0.00516	8.77000
O	18	–0.78165	1.9998	6.77630	0.00555	8.78165
C	19	–0.79258	1.99914	4.78757	0.00587	6.79258
H	20	0.26929	0.00000	0.72949	0.00122	0.73071
H	21	0.27324	0.00000	0.72584	0.00092	0.72676
H	22	0.26529	0.00000	0.73332	0.00138	0.73471
C	23	–0.20120	1.99888	4.19054	0.01179	6.20120
C	24	–0.00837	1.99895	3.99907	0.01035	6.00837
C	25	0.42250	1.99881	3.55354	0.02515	5.57750
C	26	–0.23865	1.99898	4.22991	0.00977	6.23865
C	27	–0.08136	1.99892	4.07138	0.01106	6.08136
C	28	–0.27480	1.99893	4.26322	0.01265	6.27480
C	29	–0.22406	1.99900	4.21348	0.01158	6.22406
H	30	0.23027	0.00000	0.76841	0.00132	0.76973
C	31	–0.20326	1.99897	4.19358	0.01071	6.20326
C	32	–0.17289	1.99896	4.16368	0.01024	6.17289
H	33	0.26203	0.00000	0.73618	0.00179	0.73797
C	34	–0.25245	1.99898	4.24178	0.01169	6.25245
H	35	0.24471	0.00000	0.75427	0.00102	0.75529
H	36	0.24213	0.00000	0.75659	0.00127	0.75787
H	37	0.24619	0.00000	0.75249	0.00132	0.75381
H	38	0.24601	0.00000	0.75302	0.00098	0.75399
O	39	–0.84849	1.99977	6.83997	0.00874	8.84849
Total		0.00000	71.97779	127.59174	0.43047	200.00000