Supporting Information

Revealing the supramolecular features of two Zn(II) complexes derived from a new hydrazone ligand: A combined crystallographic, theoretical and antibacterial studies

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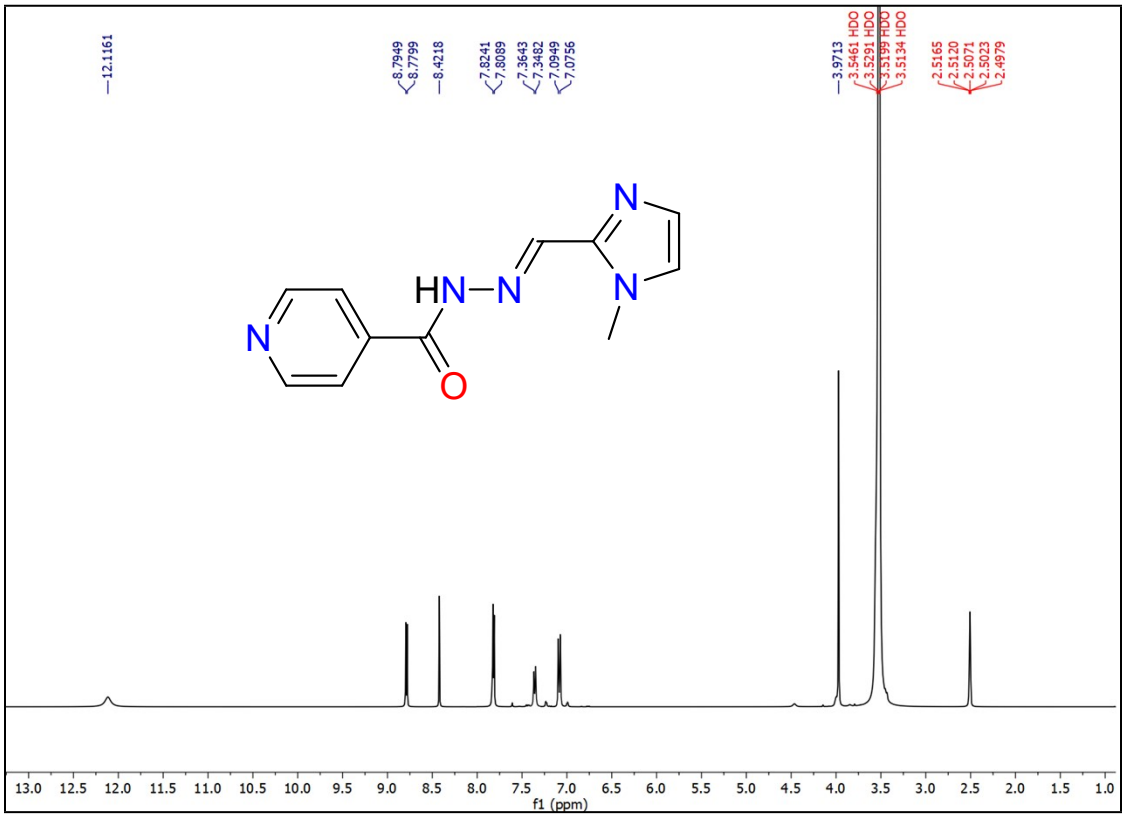

Fig. S1 ^{1}H NMR spectrum of H**L**

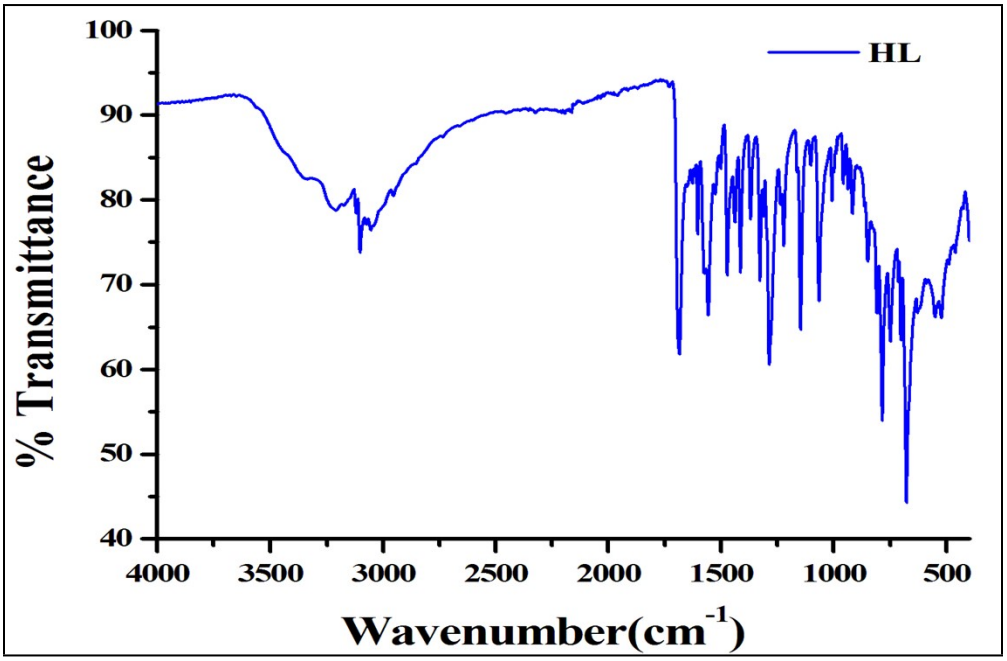

Fig. S2 FT-IR spectrum of H**L**

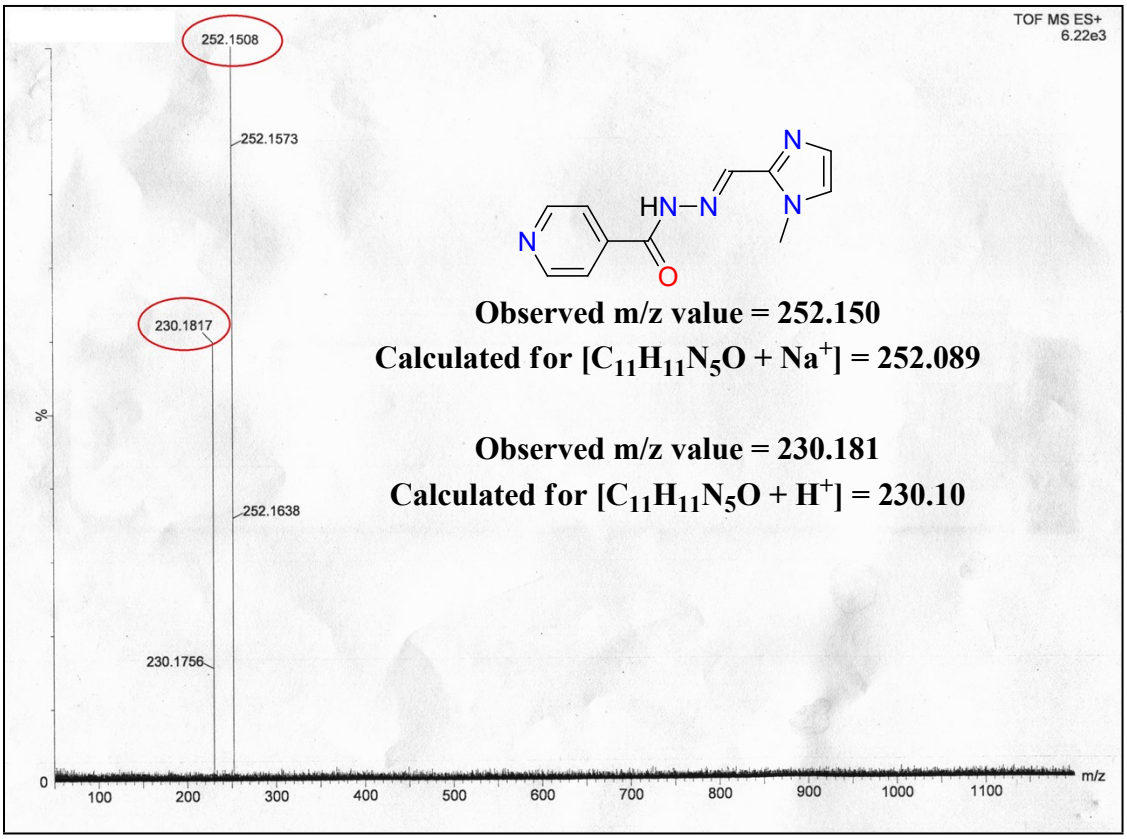

Fig. S3 ESI mass spectrum of H**L**

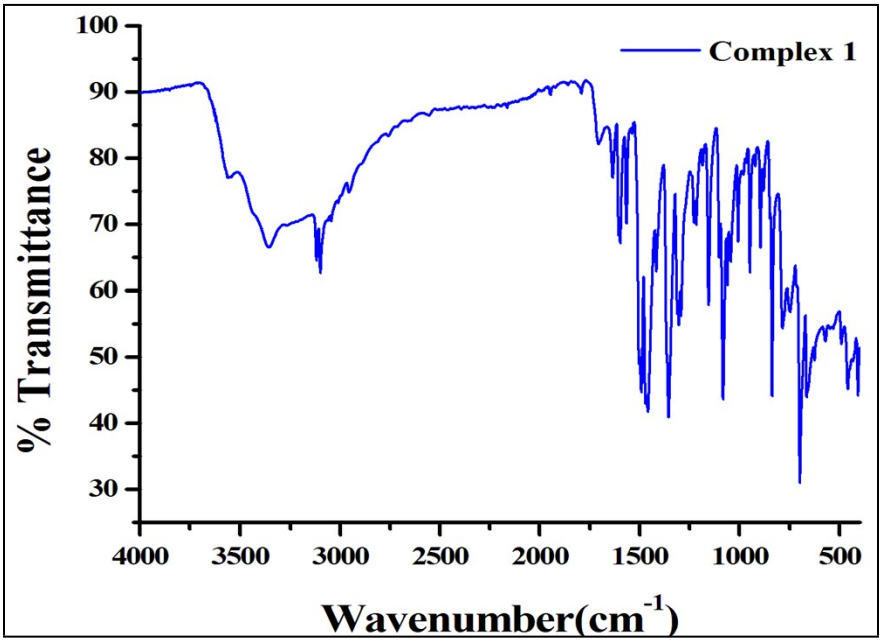

Fig. S4 FT-IR spectrum of complex **1**

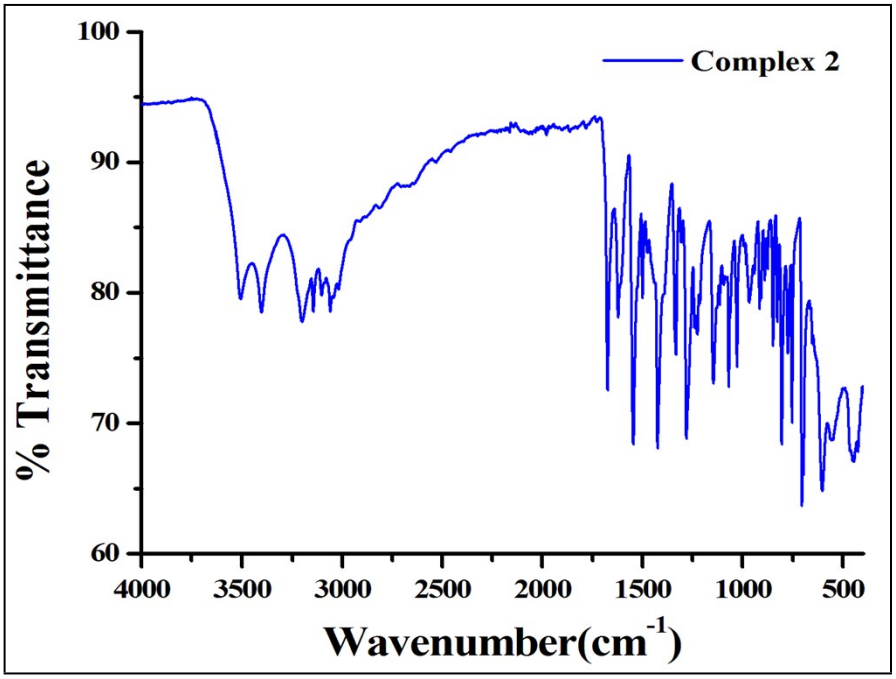

Fig. S5 FT-IR spectrum of complex **2**

Table S1 Crystal Data and Structure Refinement Parameters for Complexes 1 and 2

Structure	Complex **1**	Complex **2**
Empirical formula	$C_{22}H_{28}N_{10}O_6Zn$	$C_{11}H_{14}Cl_3N_5O_2Zn$
Formula Weight	593.93	420.01
Temperature (K)	296	296
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
space group	C2/c	P 21/c
a, b, c (Å)	23.393(5), 8.6036(19), 13.597(3)	9.473(4), 13.927(6), 13.293(5)
α, β, γ (°)	90, 107.497(7), 90	90, 105.063(5), 90
Volume (Å^3)	2610.0(10)	1693.5(12)
Z / Density (calc.) (Mg/m^3)	4 / 1.512	4 / 1.647
Absorption coefficient (mm^{-1})	0.999	1.935

F(000)	1232	848
Crystal size (mm^3)	0.08 × 0.14 × 0.19	0.09 × 0.13 × 0.19
θ range for data collection	1.833 to 27.169	2.158 to 27.842
Completeness to θ (%)	100%	100%
Absorption correction	Multi-scan	Multi-scan
Max. and min. transmission	0.923 and 0.845	0.840 and 0.747
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/parameters	2933 / 184	4022 / 203
Goodness-of-fit on F^2	0.972	0.971
Final R indices [I > 2σ(I)]	R_1 = 0.0363, wR_2 = 0.0842	R_1 = 0.0346, wR_2 = 0.0715
R indices (all data)	R_1 = 0.0573, wR_2 = 0.0880	R_1 = 0.0608, wR_2 = 0.0804
Largest diff. peak and hole ($e.Å^{-3}$)	0.387 and -0.353	0.273 and -0.339

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$, $wR_2 = [\sum\{(F_o^2-F_c^2)^2\}/\sum\{w(F_o^2)^2\}]^{1/2} w = 1/\{\sigma^2(F_o^2) + (aP)^2 + bP\}$, $P = (F_o^2 + 2F_c^2)/3$ where, a =0.0511, b =0.0 for complex **1** and a = 0.0339, b = 0.6250 for complex **2**

Table S2 Selected Bond Distances [Å] for Complexes 1 and 2

	Bonds	**Distance (Å)**	**Bonds**	**Distance (Å)**
Complex **1**	Zn1─O1	2.1877(15)	Zn1─O1_a	2.1877(15)
	Zn1─N2	2.1806(17)	Zn1─N2_a	2.1806(17)
	Zn1─N3	2.0971(17)	Zn1─N3_a	2.0971(17)
Complex **2**	Zn1─Cl1	2.2165(13)	Zn1─Cl3	2.2583(12)
	Zn1─Cl2	2.2873(12)	Zn1─N5	2.068(2)

a = 1-x,y,3/2-z

Table S3 Selected Bond Angles [°] for Complexes 1 and 2

	Bond angles	**Value (°)**	**Bond angles**	**Value (°)**
Complex **1**	O1─Zn1─N2	149.17(6)	N2─Zn1─N3_a	109.20(6)
	O1─Zn1─N3	72.42(6)	O1_a ─Zn1─N3	101.52(6)
	O1─Zn1─O1_a	97.64(5)	N2_a─Zn1─N3	109.20(6)
	O1─Zn1─N2_a	89.26(6)	N3─Zn1─N3_a	171.09(6)
	O1─Zn1─N3_a	101.52(6)	O1_a─Zn1─N2_a	149.17(6)

	N2─Zn1─N3	76.76(6)	O1_a─Zn1─N3_a	72.42(6)
	O1_a─Zn1─N2	89.26(6)	N2_a─Zn1─N3_a	76.76(6)
	N2─Zn1─N2_a	100.07(6)		
Complex **2**	Cl1─Zn1─Cl2	110.54(3)	Cl2─Zn1─Cl3	109.01(3)
	Cl1─Zn1─Cl3	119.21(3)	Cl2─Zn1─N5	101.88(6)
	Cl1─Zn1─N5	110.26(6)	Cl3─Zn1─N5	104.41(6)

a = 1-x,y,3/2-z

Table S4 Geometrical Parameters for the Hydrogen Bonds of Complexes 1 and 2

D–H···A	**D–H [Å]**	**H···A**	**D···A [Å]**	**D–H···A [°]**	**Symmetry**
Complex **1**					
O2─H2A···N5	0.8500	1.9900	2.832(2)	169.00	–
O2─H2B···O1	0.8500	2.0600	2.859(2)	157.00	x,1-y,-1/2+z
O3─H3A···O2	0.8500	2.1700	2.993(3)	162.00	1/2-x,1/2-y,-z
O3─H3B···O2	0.8500	2.0800	2.920(3)	171.00	–
C2─H2···O3	0.9300	2.5800	3.476(3)	163.00	1-x,2-y,1-z
Complex **2**					
O2─H2A···O1	0.8500	2.0500	2.879(3)	167.00	-1+x,y,z
O2─H2A···N3	0.8500	2.4700	2.982(3)	120.00	-1+x,y,z
O2─H2B···Cl3	0.8500	2.5000	3.347(3)	175.00	1-x,-1/2+y,3/2-z
N2─H2C···O2	0.8600	1.9700	2.821(3)	173.00	1+x,y,z
N4─H4C···Cl2	0.8600	2.5100	3.303(3)	154.00	1-x,-1/2+y,3/2-z
C5─H5···Cl2	0.9300	2.7200	3.526(3)	145.00	1-x,-1/2+y,3/2-z

Table S5 Geometrical Parameters (Å, °) for the π-Stacking Interactions for the Title Complexes

Cg(i)···Cg(j)	Cg(i)···Cg(j)[Å]	α (°)	β (°)	γ (°)	Cg(i)–perp[Å]	Cg(j)–perp[Å]	Symmetry
Complex **1**							
Cg(1)[1]···Cg(6)	3.8699(14)	5.38	34.13	29.52	3.367	3.203	1-x,1-y,1-z
Cg(3)[1]···Cg(6)	3.8699(14)	5.38	34.13	29.52	3.367	3.203	x,1-y,1/2+z
Cg(5)[1]···Cg(6)	3.8786(14)	11.45	25.24	36.36	3.123	3.508	1-x,2-y,1-z
Cg(6)[1]···Cg(1)	3.8699(14)	5.38	29.52	34.13	3.203	3.368	1-x,1-y,1-z
Cg(6)[1]···Cg(3)	3.8699(14)	5.38	29.52	34.13	3.203	3.368	x,1-y,-1/2+z
Cg(6)[1]···Cg(5)	3.8786(14)	11.45	36.36	25.24	3.508	3.123	1-x,2-y,1-z
Complex **2**							
Cg(1)[1]···Cg(2)	3.710(2)	8.41	29.78	21.63	3.448	3.220	2-x,-1/2+y,3/2-z
Cg(2)[1]···Cg(1)	3.710(2)	8.41	21.63	29.78	3.220	3.448	2-x,1/2+y,3/2-z

Cg(i) and Cg(j) denotes centroid of i^{th} and j^{th} ring respectively. For Complex **1**: Cg(1) is the centroid of [Zn1/O1/C6/N4/N3] ring; Cg(3) is the centroid of [Zn1/O1_a/C6_a/N4_a/N3_a] ring; Cg(5) is the centroid of [N1/C2/C3/N2/C4] ring; and Cg(6) is the centroid of [N5/C9/C8/C7/C11/C10] ring. For Complex **2**: Cg(1) is the centroid of [N1/C2/C3/N2/C4] ring and Cg(2) is the centroid of [N5/C9/C8/C7/C11/C10] ring.

Table S6. Geometrical Parameters (Å,°) for the O─H···π Interaction for the Complex 1

	X─H(I)···Cg(J)	H···Cg	X···Cg	X─H···Cg	Symmetry
Complex **1**	O(2)H(2B)─[2]···Cg(2)	2.93	3.343(2)	112	1-x,1-y,1-z
	O(2)H(2B)─[2]···Cg(4)	2.93	3.343(2)	112	x,1-y,-1/2+z

For Complex **1**: Cg(2) is the centroid of [Zn1/N2/C4/C5/N3] ring and Cg(4) is the centroid of [Zn1/N2_a/C4_a/C5_a/N3_a] ring.

Table S7. Geometrical Parameters (Å, °) for the Anion···π/Lone Pair···π Interactions for the Complex 2

	Y–X(I)···Cg(J)	X···Cg [Å]	Y···Cg [Å]	Y–X···Cg (°)	Symmetry
Complex **2**	Zn(1)─Cl(3)[1]···Cg(2)	3.608(2)	4.622(2)	101.49(3)	1-x,2-y,1-z
	C(6)─O(1)[1]···Cg(1)	3.186(3)	3.320(3)	85.49(15)	2-x,1-y,1-z

For Complex **2**: Cg(1) is the centroid of [N1/C2/C3/N2/C4] ring and Cg(2) is the centroid of [N5/C9/C8/C7/C11/C10] ring.

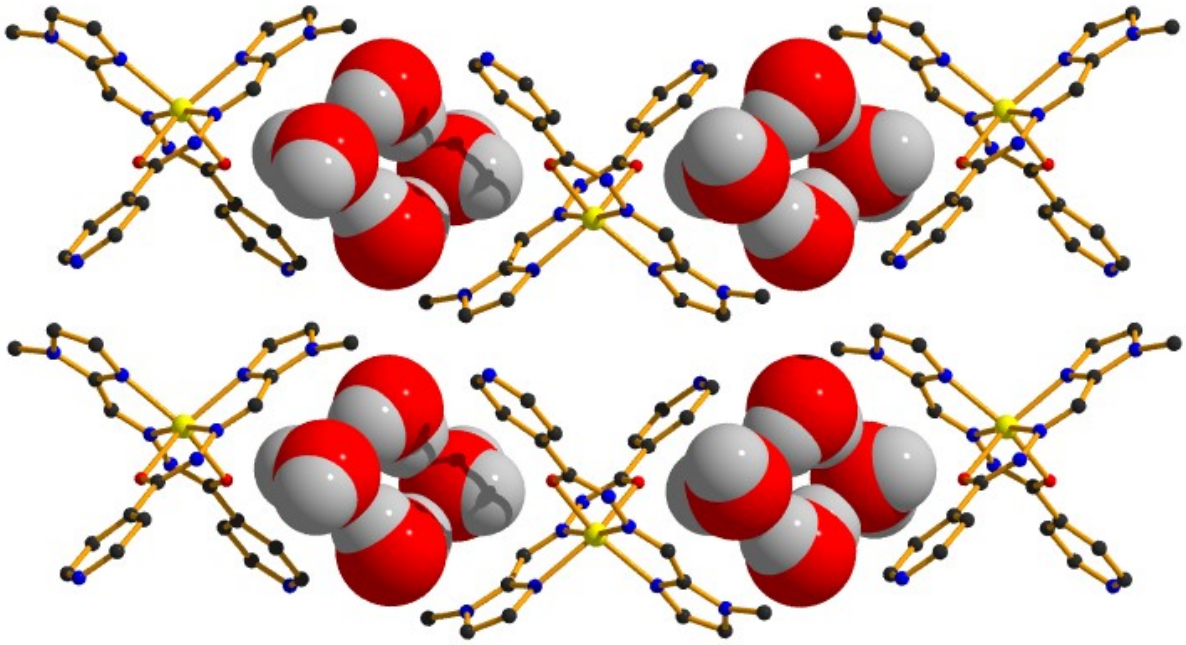

Fig. S6 Filling of void spaces through water cluster present in complex **1**