Supplementary Information (SI) for RSC Advances.

Supplementary data

Integrated Structural, Vibrational, Thermal, and Optical Characterization of a Zinc-Based Organic–Inorganic Hybrid with DFT and Molecular Docking Insights into Its Biological Properties

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Table S1. Experimental conditions and data collection of the $(C_9H_8N)_2[ZnCl_4]\cdot 2H_2O$ crystal.

Formula	$(C_9H_8N)_2[ZnCl_4]\cdot 2H_2O$
Color/Shape	Plate, colorless
M ($gmol^{-1}$)	503.53
Crystal system	Monoclinic
Space group	*C2/c*
Density	1.602
Crystal size (mm)	0.18 × 0.13 × 0.04
Temperature (K)	100
Diffractometer	Xcalibur. Atlas. Gemini ultra
a, *b*, *c (Å)*	11.7276 (3), 9.8806 (2), 18.3798 (4)
β (°)	101.355 (2)
Unit-cell volume $(Å)^3$	2088.08 (8)
Z	4
Radiation type	Mo *Kα* (0.71073 Å)
Absorption correction	Multi-scan
θ (°)	$2.7 \leq \theta \leq 30.7$
No. of measured, independent, and observed [$I > 2\sigma(I)$] reflections	23309, 2856, 2570
Index ranges	h = −16/16. k = -14/13. l = -26/25
$(\Delta/\sigma)_{max}$	= 0.001
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.021, 0.051, 1.06
F(000)	1024
$\Delta\rho_{max}$ /$\Delta\rho_{min}$ (e $Å^{-3}$)	0.35 /−0.26

Table S2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	y	z	Uiso*/Ueq
Zn1	0.500000	0.84465 (2)	0.750000	0.01398 (6)
Cl1	0.65065 (3)	0.71237 (3)	0.80803 (2)	0.02032 (7)
Cl2	0.57264 (3)	0.97068 (3)	0.66770 (2)	0.02047 (7)
O1	0.34922 (8)	0.39959 (10)	0.72508 (5)	0.02215 (19)
H1B	0.276731	0.380104	0.724628	0.033*
H1C	0.351339	0.487625	0.724835	0.033*
N1	0.43774 (9)	0.34680 (10)	0.60066 (6)	0.0169 (2)
H1	0.408831	0.363809	0.640410	0.020*
C1	0.54303 (11)	0.29337 (13)	0.60954 (7)	0.0187 (2)
H1A	0.585369	0.274596	0.658082	0.022*
C2	0.59248 (11)	0.26433 (13)	0.54800 (7)	0.0196 (2)
H2	0.668189	0.226242	0.554504	0.023*
C3	0.53060 (11)	0.29139 (12)	0.47834 (7)	0.0176 (2)
H3	0.563433	0.271471	0.436260	0.021*
C4	0.41800 (11)	0.34884 (12)	0.46847 (7)	0.0150 (2)
C5	0.34896 (12)	0.37795 (13)	0.39785 (7)	0.0184 (2)
H5	0.378340	0.359975	0.354208	0.022*
C6	0.24009 (12)	0.43189 (13)	0.39234 (7)	0.0206 (3)
H6	0.194272	0.450920	0.344808	0.025*
C7	0.19524 (11)	0.45950 (13)	0.45670 (8)	0.0204 (3)
H7	0.119544	0.497043	0.451867	0.025*
C8	0.25926 (11)	0.43297 (13)	0.52601 (7)	0.0180 (2)
H8	0.228698	0.451939	0.569100	0.022*
C9	0.37128 (10)	0.37703 (12)	0.53214 (7)	0.0149 (2)

Table S3. Geometric parameters (Å, °).

Distances	
Zn1—Cl1i	2.2859 (3)
Zn1—Cl1	2.2858 (3)
Zn1—Cl2	2.2521 (3)
Zn1—Cl2i	2.2520 (3)
O1—H1B	0.8701
O1—H1C	0.8702
N1—H1	0.8800
N1—C1	1.3231 (17)
N1—C9	1.3771 (16)
C1—H1A	0.9500
C1—C2	1.3986 (18)
C2—H2	0.9500
C2—C3	1.3681 (18)
C3—H3	0.9500
C3—C4	1.4158 (17)
C4—C5	1.4174 (17)
C4—C9	1.4141 (16)
C5—H5	0.9500
C5—C6	1.3688 (19)
C6—H6	0.9500
C6—C7	1.4125 (19)
C7—H7	0.9500
C7—C8	1.3707 (18)
C8—H8	0.9500
C8—C9	1.4093 (17)
Angles	
Cl1—Zn1—Cl1i	110.252 (19)
Cl2—Zn1—Cl1i	111.258 (11)
Cl2i—Zn1—Cl1	111.260 (11)
Cl2—Zn1—Cl1	105.647 (11)

Cl2i—Zn1—Cl1i	105.647 (11)
Cl2i—Zn1—Cl2	112.863 (19)
H1B—O1—H1C	104.5
C1—N1—H1	118.5
C1—N1—C9	123.07 (11)
C9—N1—H1	118.5
N1—C1—H1A	119.7
N1—C1—C2	120.50 (11)
C2—C1—H1A	119.7
C1—C2—H2	120.4
C3—C2—C1	119.26 (12)
C3—C2—H2	120.4
C2—C3—H3	119.7
C2—C3—C4	120.52 (11)
C4—C3—H3	119.7
N1—C1—C2—C3	−0.20 (19)
C1—N1—C9—C4	0.30 (18)
C1—N1—C9—C8	179.54 (11)
C1—C2—C3—C4	0.35 (19)
C2—C3—C4—C5	−179.31 (12)
C2—C3—C4—C9	−0.18 (18)
C3—C4—C5—C6	179.12 (12)
C3—C4—C9—N1	−0.14 (17)
C3—C4—C9—C8	−179.37 (11)
Cl1—Zn1—Cl1i	110.252 (19)
Cl2—Zn1—Cl1i	111.258 (11)
Cl2i—Zn1—Cl1	111.260 (11)
Cl2—Zn1—Cl1	105.647 (11)
Cl2i—Zn1—Cl1i	105.647 (11)
Cl2i—Zn1—Cl2	112.863 (19)
H1B—O1—H1C	104.5
C1—N1—H1	118.5
C1—N1—C9	123.07 (11)

C9—N1—H1	118.5
N1—C1—H1A	119.7
N1—C1—C2	120.50 (11)
C2—C1—H1A	119.7
C1—C2—H2	120.4
C3—C2—C1	119.26 (12)
C3—C2—H2	120.4
C2—C3—H3	119.7
C2—C3—C4	120.52 (11)
C4—C3—H3	119.7
N1—C1—C2—C3	−0.20 (19)
C1—N1—C9—C4	0.30 (18)
C1—N1—C9—C8	179.54 (11)
C1—C2—C3—C4	0.35 (19)
C2—C3—C4—C5	−179.31 (12)
C2—C3—C4—C9	−0.18 (18)
C3—C4—C5—C6	179.12 (12)
C3—C4—C9—N1	−0.14 (17)
C3—C4—C9—C8	−179.37 (11)

Symmetry code: (i) −x+1, y, −z+3/2.

Table S4. Hydrogen bonds in $(C_9H_8N)_2[ZnCl_4]\cdot 2H_2O$.

D—H···A	**D—H (Å)**	**H···A (Å)**	**D···A (Å)**	**D—H···A (°)**
O_1—H_{1B}···Cl_2^{ii}	0.87	2.58	3.283	139
O_1—H_{1C}···Cl_1^{i}	0.87	2.30	3.1498 (11)	165
N_1—H_1···O_1	0.88	1.86	2.7412 (14)	179

Symmetry codes : (i) −*x*+1, *y*, −*z*+3/2; (ii) *x*−1/2, *y*−1/2, *z*.

Table S5. Geometric parameters of π–π and C–H···π interactions

Interaction	Centroid–centroid distance (Å)	Interplanar distance (Å)	Slippage angle (°)
π–π (Cg···Cg)	3.698	3.365	1.05
π–π (Cg···Cg)	3.690	3.478	2.28
C–H···π	3.370	3.365	1.07

Table S6. IR and Raman frequencies (cm^{-1}) and band assignments for $(C_9H_8N)_2[ZnCl_4]\cdot 2H_2O$.

IR	Raman	Assignements
3485	-	ν(O−H)
3394	-	ν_{as}(C−H)
-	3195	ν(N−H)
3087	-	ν(C=N)
3038	3060	ν(C=C)
2667	-	δ(C−H)
-	2470	ν(C−N)
2130	2149	νin−plane(Ring)
2004	1978	ρ(C−H)
1648	-	ν(Pd−O)
-	1878	ν(Pd−Cl)
1600	1600	δ(Framework)
1488	1491	δ(Pd−Cl)
1383	1382	ν_{as}(Pd−Cl)
1313	-	β(Pd−O−Cl)
-	1057	τ(Framework)
1215	-	β(Lattice)
1062	-	β(Lattice)
949	-	τ(Framework)
810	-	β(Lattice)
761	772	δ(Pd−Cl)
608	-	τ(Framework)
517	521	ν_{as}(Pd−Cl)
454	-	τ(Framework)
-	104	ν_s(Pd−Cl)
-	75	β(Lattice)
-	52	β(Lattice)

ν:stretching, ν_{as}: assymetric stretching, β: in plane bending, δ: scissoring, $\mathcal{T}$:twisting, ρ:rocking

Table S7. Quantum Chemical Parameters of Zn Complex of zinc complex.

Parameter	**Zn Complex**
HOMO (eV)	−12.32
LUMO (eV)	−7.48
Energy Gap, Eg (eV)	4.84
Optical Band Gap (eV)	4.84
Dipole Moment (D)	10.45
SCF Energy (eV)	−4801.86
Chemical Potential, μ (eV)	−9.90
Electronegativity, χ (eV)	9.90
Chemical Hardness, η (eV)	2.42
Softness, S (eV^{-1})	0.207
Electrophilicity Index, ω (eV)	20.25

Table S8. Predicted Physicochemical and ADME Properties of Ciprofloxacin and zinc complex.

Parameter Category	**Property**	**Ciprofloxacin**	**Zinc Complex**
Physicochemical	Molecular Weight (g/mol)	331.34	503.56
	TPSA ($Å^2$)	74.57	46.74
Lipophilicity	Consensus Log P	1.10	3.46
Water Solubility	Ali Log S (Class)	0.00 (Highly Soluble)	−7.26 (Poorly Soluble)
Pharmacokinetics	GI Absorption	High	High
	BBB Permeant	No	No
	P-gp Substrate	Yes	Yes
Drug-likeness	Lipinski Violations	0	1 (MW > 500)
	Veber Violations	0	0
	Bioavailability Score	0.55	0.55
Synthesis	Synthetic Accessibility	2.51	2.23

Table S9. Absorption Properties (pkCSM Prediction) for Zn Complex.

Property Category	Model Name	Predicted Value
Absorption	Water Solubility (log mol/L)	−3.774
	Caco-2 Permeability (log Papp in 10^{-6} cm/s)	0.623
	Intestinal Absorption (Human, %)	91.607
	Skin Permeability (log Kp)	−2.704
	P-glycoprotein (P-gp) Substrate	No
	P-gp I Inhibitor	Yes
	P-gp II Inhibitor	Yes

Table S10. Molecular Docking of Ciprofloxacin and Zn complex with DNA Gyrase (PDB: 1AB4).

Ligand	Ligand Sites	Receptor Sites	Type of Interaction	Distance (Å)	Binding Energy (kcal/mol)	Total Binding Energy (kcal/mol)
Ciprofloxacin	N29	ASP87 (A)	H-bond (donor)	2.96	−0.9	−6.13
	O41	VAL268 (A)	H-bond (donor)	2.75	−2.3	
Zn complex	6-ring	PHE96 (A)	π–H interaction	4.15	−0.6	−4.96
	6-ring	GLN267 (A)	π–H interaction	4.12	−0.6	

Table S11. Molecular Docking of Ciprofloxacin and Zn complex with LasR (PDB: 3IX3).

Ligand	Ligand Sites	Receptor Sites	Type of Interaction	Distance (Å)	Binding Energy (kcal mol^{-1})	Total Binding Energy (kcal mol^{-1})
Ciprofloxacin	O1	TRP60 (A)	H-acceptor	3.29	−1.7	−7.68
Zn complex	CL5	TYR47 (A)	H-donor	3.15	−2.4	−5.88
	6-ring	TYR64 (A)	π–π stacking	3.60	~0.0	