

Supplementary data

Structure–Biological Activity Relationships in a Zinc(II) Pyrazole Halide Complex $[\text{ZnCl}_2(\eta^1\text{-4BrPz})_2]$ via Noncovalent Interactions, Molecular Docking, and Antimicrobial Studies

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Table.S1. Experimental conditions and data collection of the $[\text{ZnCl}_2(\eta^1\text{-4BrPz})_2]$ crystal.

Formula	$[\text{ZnCl}_2(\text{C}_3\text{H}_3\text{BrN}_2)_2]$
Color/Shape	Colorless/Block-shaped
Mr (gmol⁻¹)	430.24
Crystal system	Monoclinic
Space group	<i>P2/c</i>
Density	2.439
Crystal size (mm)	0.27 × 0.17 × 0.09
Temperature (K)	100
Diffractometer	Xcalibur. Atlas. Gemini ultra
<i>a, b, c</i> (Å)	21.3691 (3), 4.0847 (1), 14.2396 (2)
<i>β</i> (°)	109.475 (2)
Unit-cell volume (Å³)	1171.81 (4)
<i>Z</i>	4
Radiation type	Mo <i>Kα</i> (0.71073 Å)
Absorption Correction	multi-scan
<i>θ</i> (°)	2.9 ≤ <i>θ</i> ≤ 30.4
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	29781, 3220, 3128
Index ranges	<i>h</i> = -29/28. <i>k</i> = -5/5. <i>l</i> = -19/19
(Δ/σ)_{max}	= 0.002
R[<i>F</i>² > 2σ(<i>F</i>²)], wR(<i>F</i>²), <i>S</i>	0.025, 0.063, 1.04
<i>F</i>(000)	816
Δρ_{max} / Δρ_{min} (e Å⁻³)	1.11/ -1.00

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.77385 (2)	0.48101 (8)	0.75810 (3)	0.01445 (8)
Zn1	0.500000	0.75326 (12)	0.750000	0.01363 (11)
Cl1	0.44451 (3)	1.02812 (18)	0.60590 (6)	0.01548 (14)
N1	0.57820 (13)	0.5630 (7)	0.71894 (19)	0.0128 (5)
N2	0.57659 (14)	0.4008 (7)	0.63501 (19)	0.0146 (5)
H2	0.539851	0.340403	0.588036	0.018*
C00I	0.63783 (18)	0.3436 (8)	0.6323 (3)	0.0171 (7)
H00I	0.648989	0.230976	0.581709	0.021*
C1	0.64238 (16)	0.6169 (8)	0.7693 (2)	0.0143 (6)
H1	0.658983	0.730600	0.830817	0.017*
C2	0.68130 (12)	0.4809 (7)	0.7177 (3)	0.0119 (5)
Br2	0.73676 (2)	-0.19273 (7)	0.49343 (2)	0.01462 (8)
Zn2	1.000000	0.31780 (11)	0.750000	0.01026 (10)
Cl2	1.05138 (3)	0.56159 (16)	0.65174 (6)	0.01316 (13)
N3	0.92389 (13)	0.1184 (7)	0.63981 (18)	0.0116 (5)
N4	0.92164 (14)	0.1348 (7)	0.54382 (19)	0.0129 (5)
H4	0.954658	0.203508	0.524997	0.016*
C3	0.86274 (18)	0.0334 (8)	0.4807 (3)	0.0157 (7)
H3	0.849639	0.023588	0.410102	0.019*
C4	0.82501 (12)	-0.0541 (6)	0.5392 (3)	0.0112 (5)
C5	0.86522 (17)	0.0026 (7)	0.6376 (2)	0.0109 (6)
H5	0.852528	-0.035893	0.694547	0.013*

Table S3. Atomic displacement parameters (\AA^2).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.00919 (13)	0.01884 (14)	0.01605 (17)	0.00121 (10)	0.00519 (16)	0.00237 (11)
Zn1	0.0075 (2)	0.0196 (2)	0.0137 (3)	0.000	0.0034 (2)	0.000
Cl1	0.0099 (3)	0.0212 (3)	0.0140 (4)	-0.0023 (2)	0.0023 (3)	0.0014 (3)
N1	0.0106 (13)	0.0165 (12)	0.0106 (12)	0.0005 (10)	0.0024 (10)	-0.0001 (10)
N2	0.0110 (13)	0.0220 (13)	0.0096 (12)	-0.0033 (11)	0.0018 (10)	-0.0042 (10)
C00I	0.0173 (17)	0.0177 (16)	0.0162 (16)	0.0000 (12)	0.0055 (14)	-0.0012 (12)
C1	0.0118 (15)	0.0152 (14)	0.0145 (15)	-0.0016 (11)	0.0026 (12)	-0.0014 (11)
C2	0.0085 (11)	0.0133 (12)	0.0143 (15)	0.0012 (9)	0.0042 (14)	0.0040 (10)
Br2	0.00964 (13)	0.01978 (14)	0.01305 (15)	-0.00374 (9)	0.00194 (13)	-0.00064 (11)
Zn2	0.0079 (2)	0.0158 (2)	0.0072 (2)	0.000	0.00263 (19)	0.000

CI2	0.0117 (3)	0.0192 (3)	0.0099 (3)	-0.0031 (2)	0.0053 (3)	0.0007 (3)
N3	0.0124 (14)	0.0167 (12)	0.0068 (12)	0.0003 (10)	0.0047 (10)	0.0016 (9)
N4	0.0128 (13)	0.0192 (13)	0.0065 (12)	-0.0039 (10)	0.0030 (10)	-0.0013 (10)
C3	0.0138 (16)	0.0212 (16)	0.0107 (15)	-0.0030 (12)	0.0022 (13)	-0.0014 (12)
C4	0.0087 (11)	0.0135 (13)	0.0108 (13)	-0.0010 (9)	0.0026 (12)	0.0009 (12)
C5	0.0097 (15)	0.0133 (14)	0.0097 (14)	0.0013 (10)	0.0031 (12)	0.0005 (10)

Table S4. Docking scores and interaction details of the interaction between $[\text{ZnCl}_2(\eta^1\text{-4BrPz})_2]$ and the target.

Microorganism		ID	X;Y;Z coordinates	Docking affinity (kcal/mole)	Type of Hydrogen Bond	Residue	Distance (Å)
Staphylococcus aureus	Gyrase A	P20831	10.660; -10.313; 2.388	-4.3	conventional	ASP114	2.44
					conventional	THR296	2.29
	Gyrase B	P0A0K8	-13.098; 2.588; 31.162	-4.5	conventional	TYR117	2.58
					conventional	TYR117	2.49
					carbon	GLY339	3.40
Bacillus cereus	Gyrase A	A0A1S9UZ55	-38.525; -10.909; 49.205	-4.1	conventional	ASP543	2.35
	Gyrase B	Q9X3Y3	-30.256; -8.696; 1.954	-4.7	conventional	GLY378	3.08
Enterococcus faecalis	Gyrase A	A0A1J6YID4	15.342; 7.464; -25.976	-3.9	conventional	GLU55	2.28
					conventional	ILE139	2.98
					conventional	ASN140	2.41
	Gyrase B	Q839Z1	33.127; 8.561; 2.489	-4.9	π -donor	GLN85	2.74
Micrococcus luteus	Gyrase	C5C7X9	9.348;	-3.6	carbon	MET73	3.79

	e A		2.288; -62.229			2	
	Gyras e B	C5C7X8	17.617; 26.649; -1.145	-4.4	carbon	GLU89	3.26
carbon					GLY147	3.01	
carbon					GLY116	3.66	
Escherichia coli							
	Gyras e A	POAES4	234.321; 247.599; 254.078	-3.1	conventional	ASP137	2.62
					carbon	GLU139	3.53
	Gyras e B	POAES6	251.824; 269.940; 202.136	-5.3	conventional	ASP49	3.00
Pseudomonas aeruginosa							
	Gyras e A	P48372	255.147; 187.948; 268.815	-4.6	conventional	ALA656	2.40
					conventional	VAL674	2.58
	Gyras e B	Q9I7C2	-1.836; -10.457; -6.097	-4.6	conventional	ILE769	2.76
					conventional	GLU770	2.83
					carbon	ARG278	3.70
Klebsiella pneumoniae							
	Gyras e A	A0A9Q6A465	235.850; 186.618; 255.497	-4.1	carbon	ASN318	3.70
	Gyras e B	A0A377VTL4	275.164; 263.511; 209.317	-3.7			
Salmonella enterica							
	Gyras e A	A0A3Y8V8W7	233.975; 247.967; 246.628	-4.2			
	Gyras e B	A0A3Z4CPQ3	177.888; 248.713; 270.155	-4.5	Carbon	HIS99	3.22
Salmonella typhi							
	Gyras e A	A6GVE9	200.955; 257.295; 229.286	-4.1	conventional	VAL143	2.97
					carbon	GLU141	3.46
	Gyras e B	P0A2I4	177.888; 248.713; 270.155	-4.5	carbon	HIS83	3.77
					carbon	HIS99	3.24
Aspergillus niger		A2QC57	8.966; 44.430; 6.100	-4.7	conventional	THR60	2.82
					conventional	THR60	1.82

					al		
					carbon	THR58	3.59
Candida albicans		P30573	14.095; -32.011; 4.101	-4.1	conventional	GLU16	2.60
					π -donor	SER21	2.63

Table S5. IR and Raman frequencies (cm⁻¹) and band assignments for [ZnCl₂(η¹-4BrPz)₂]

<i>IR</i>	<i>Raman</i>	<i>Assignment</i>
3336	3342	$\nu_s(\text{N-H})$
3129	3161	$\nu_{as}(\text{C-H})$
-	3135	$\nu_{as}(\text{C-H})$
1618	-	$\nu(\text{C=N})$
1523	1466	$\nu(\text{C=C})$
1427	-	$\delta(\text{C-H})$
1388	-	$\nu(\text{C-C})$
1332	-	$\nu(\text{C-N})$
1255	-	$\nu(\text{C-Br})$
1194	1192	$\nu(\text{C-Cl})$
1125	1125	$\nu(\text{Zn-N})$
1048	-	$\nu(\text{Zn-Cl})$
-	1004	$\nu_s(\text{Ring})$
-	958	$\beta(\text{Ring})$
950	-	$\gamma(\text{C-H})$
875	-	$\nu_{as}(\text{Zn-Cl})$
856	-	$\nu_{as}(\text{Zn-Cl})$
846	-	$\nu_{as}(\text{Zn-Cl})$
829	-	$\nu(\text{Zn-Br})$
660	-	$\beta(\text{Framework})$
573	-	$\beta(\text{Zn-Br, Ligand})$
424	-	$\nu(\text{Metal-Ligand})$
-	258	$\tau(\text{Framework})$
-	155	$\tau(\text{Framework})$
-	131	$\tau(\text{Framework})$
-	81	$\nu_s(\text{N-H})$

ν_s : symmetric stretching, ν_{as} : asymmetric stretching, β : in plane bending, δ : scissoring, \mathcal{T} : twisting, ρ : rocking.

Table S6. Antibacterial activity of $[\text{ZnCl}_2(\eta^1\text{-4BrPz})_2]$ and tetracycline against eight bacterial strains.

	Compound concentration ($\mu\text{g/mL}$)	Zone of inhibition (mm)	Tetracyclin (1 $\mu\text{g/mL}$)
<i>Enterococcus faecalis</i>	0.5	7.2	19.8
	1	12.9	
	2	17.8	
<i>Escherichia coli</i>	0.5	11.4	21.4
	1	19.4	
	2	24.3	
<i>Bacillus cereus</i>	0.5	9.4	22.8
	1	17.8	
	2	24.6	
<i>Pseudomonas aeruginosa</i>	0.5	6.3	6.6
	1	11.1	
	2	17.8	
<i>Staphylococcus aureus</i>	0.5	4.2	23.2
	1	7.8	
	2	12.3	
<i>Salmonella enterica</i>	0.5	4.8	17.8
	1	8.6	
	2	15.2	
<i>Salmonella typhi</i>	0.5	3.9	16.8
	1	6.4	
	2	9.8	
<i>Micrococcus luteus</i>	0.5	5.4	22.4
	1	10.2	
	2	17.2	

Table S7: Comparative MIC and MBC values of $[\text{ZnCl}_2(\eta^1\text{-4BrPz})_2]$ and its free ligand (4BrP) against selected bacterial strains.

Bacterial strain	$\text{ZnCl}_2(\eta^1\text{-4BrPz})_2$			Ligand (4BrP)		
	MIC ($\mu\text{g/mL}$)	MBC ($\mu\text{g/mL}$)	MBC/MIC ratio	MIC ($\mu\text{g/mL}$)	MBC ($\mu\text{g/mL}$)	MBC/MIC ratio
<i>Enterococcus faecalis</i>	0.94	1.89	2.01	3.32	13.9	4.18
<i>Escherichia coli</i>	0.45	0.87	1.93	3.19	12.8	4.01
<i>Bacillus cereus</i>	0.72	1.32	1.83	4.41	13.2	2.99
<i>Pseudomonas aeruginosa</i>	1.94	3.12	1.61	7.84	19.76	2.52
<i>Staphylococcus aureus</i>	1.55	2.19	1.41	3.89	16.34	4.20
<i>Salmonella enterica</i>	1.64	2.59	1.58	3.32	13.89	4.18
<i>Salmonella typhi</i>	2.1	3.74	1.78	3.84	17.44	4.54
<i>Micrococcus luteus</i>	0.89	1.62	1.82	2.89	11.70	4.04