Electronic Supplementary Material (ESI) for New Journal of Chemistry.

A new model of metalloantibiotic: Synthesis, structure and biological activity of a zinc(II) mononuclear complex carrying two enrofloxacin and sulfadiazine antibiotics

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SUPPLEMENTARY INFORMATION

SINGLE-CRYSTAL X-RAY DIFFRACTION CHARACTERIZATIONS

Table SI.1. Single-crystal X-ray diffraction data and crystal structure refinement results for complexes (**1)** and (**3)**.

	(1)	**(3)**
Formula	$C_{20}H_{23}N_9O_5S_2Zn_1$	$C_{48}H_{53}Cl_1F_2N_{10}O_{12}S_1Zn_1$
Molecular weight (g.mol^{-1})	598.97	1132.90
Temperature (K)	293	293
Crystal system	Orthorhombic	Triclinic
Space group	$Pna2_1$	P-1
Flack parameter	0.11(2)	-
Crystal shape	prismatic	needle
Crystal color	colorless	colorless
Crystal size (mm^3)	0.11×0.11×0.11	0.09×0.35×0.50
Density	1.591	1.540
μ (mm^{-1})	1.201	0.683
a (Å)	13.898(2)	12.6714(6)
b (Å)	12.655(3)	14.1042(7)
c (Å)	14.221(3)	15.0668(7)
α (deg.)	90	68.569(5)
β (deg.)	90	81.395(4)
γ (deg.)	90	77.993(4)
V (Å^3)	2501.0(9)	2443.7(2)
Z	4	2
No. refl. / unique refl. / R_{int}	7690 / 4563 / 0.029	23105 / 11457 / 0.039
R(F) / R_w(F)	0.0508 / 0.0660	0.0966 / 0.0938
S	1.06	1.02
No. refl. used	3458	6733
No. refined parameters	335	677
Electronic residue (e$^-$.Å^{-3})	-0.82 / +0.32	-2.20/+ 1.41
Absorption correction	Analytical	Analytical

Table SI.2. Important bond lengths (Å), angles (°) and distances (Å) within structure of complex **(1)**.

Zn1-N7	2.185(5)	Zn1-N21	2.081(4)	Zn1-N27	2.738(5)
Zn1-N41	2.049(5)	Zn1-O42	2.034(6)	Zn1-N1	2.413(5)
N1-Zn1-N7	58.4(2)	N1-Zn1-N21	89.7(2)	N7-Zn1-N21	97.4(2)
N1-Zn1-N27	143.3(2)	N7-Zn1-N27	124.9(2)	N21-Zn1-N27	54.0(2)
N1-Zn1-N41	138.7(2)	N7-Zn1-N41	93.2(2)	N21-Zn1-N41	126.0(2)
N27-Zn1-N41	76.7(2)	N1-Zn1-O42	87.0(2)	N7-Zn1-O42	136.6(2)
N21-Zn1-O42	108.6(2)	N27-Zn1-O42	98.5(2)	N41-Zn1-O42	98.4(2)

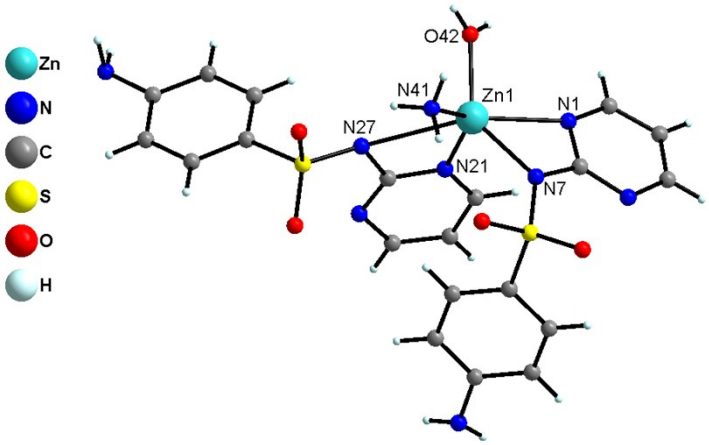

Figure SI.1. Complex **(1)** with important labels.

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Table SI.3. Important bond lengths (Å), angles (°) and distances (Å) within structure model of complex **(2)**.

Zn1-O2	2.118(2)	Zn1-O2	2.121(2)	Zn1-O10	2.044(2)
O2-Zn1-O2	84.47(9)	O2-Zn1-O10	85.51(8)	O2-Zn1-O10	95.96(8)
O2-Zn1-O10	169.88(8)	O10-Zn1-O10	94.16(8)		

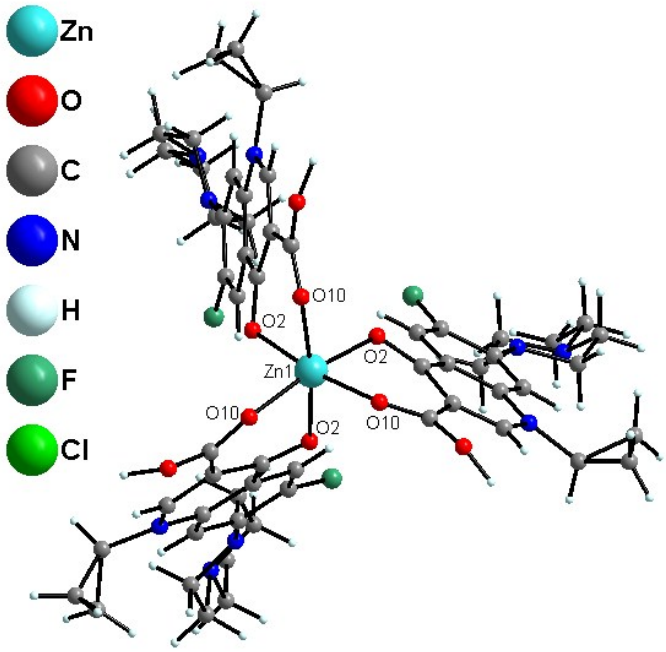

Figure SI.2. Structure model of complex **(2)** with important labels.

Table SI.4. Important bond lengths (Å), angles (°) and distances (Å) within structure of complex **(3)**.

Zn1-O2	2.124(4)	Zn1-O10	1.983(4)	Zn1-O29	2.006(5)
Zn1-O50	2.052(4)	Zn1-N55	2.045(5)		
O2-Zn1-O10	87.2(2)	O2-Zn1-O29	90.4(2)	O10-Zn1-O29	107.6(2)
O2-Zn1-O50	175.3(2)	O10-Zn1-O50	89.1(2)	O29-Zn1-O50	88.0(2)
O2-Zn1-N55	85.4(2)	O10-Zn1-N55	145.0(2)	O29-Zn1-N55	106.6(2)
O50-Zn1-N55	99.3(2)				

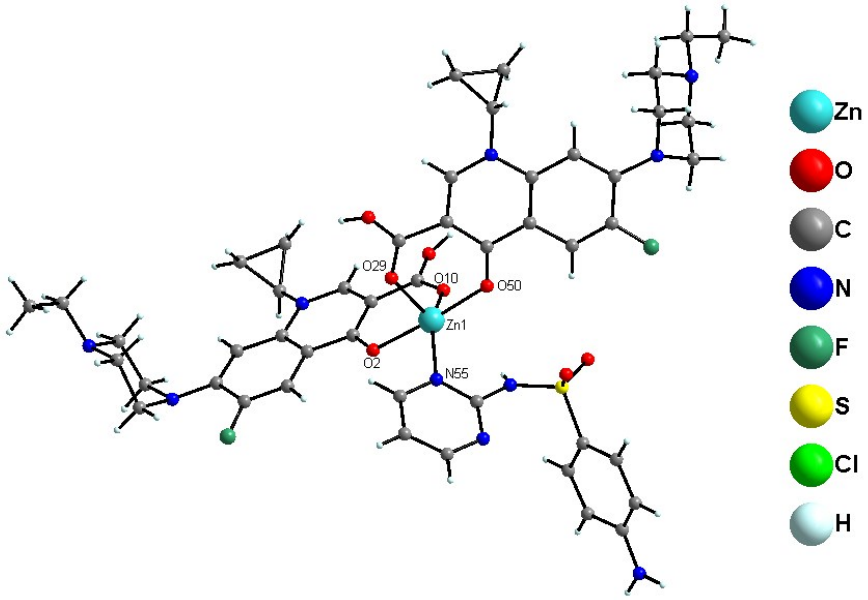

Figure SI.3. Complex **(3)** with important label

POWDER DIFFRACTION CHARACTERIZATIONS

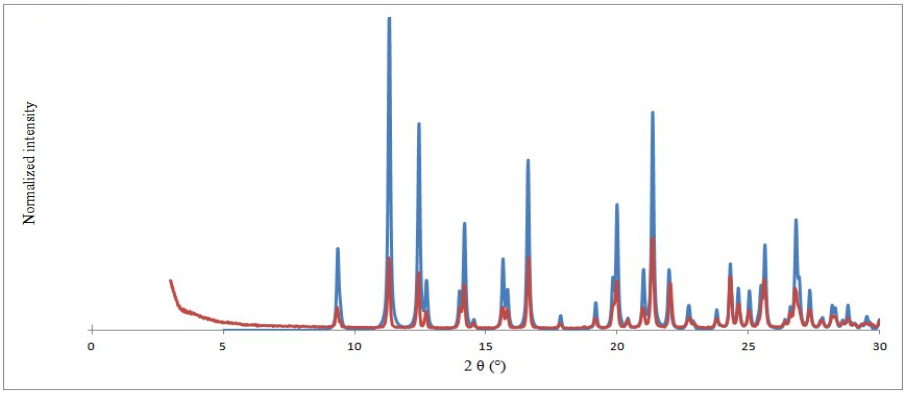

Figure SI-4. Powder diffraction pattern highlighting sample purity of complex **(1).** Red line : observed pattern, blue line: calculated pattern.

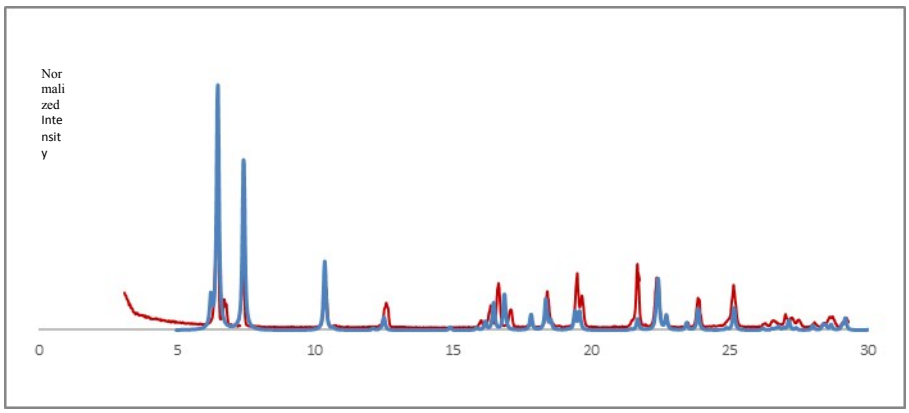

Figure SI-5. Powder diffraction pattern highlighting sample purity of complex **(2).** Red line : observed pattern, blue line: calculated pattern.

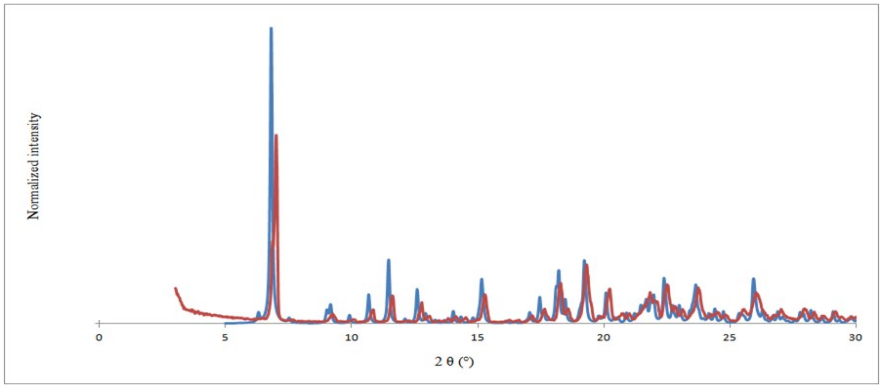

Figure SI-6. Powder diffraction pattern highlighting sample purity of complex **(3).** Red line : observed pattern, blue line: calculated pattern.

Table SI–5 : ^{1}H NMR data (600 MHz, DMSO-d_6)

Sulfadiazine : δ = 5.93 (s, 2H), δ = 6.56 (d, J = 8.7 Hz, 2H), δ = 6.99 (t, J = 5 Hz, 1H), δ = 7.61 (d, J = 8.7 Hz, 2H), δ = 8.47 (d, J = 5 Hz, 2H), δ = 11.15 (s, 1H)

Enrofloxacin : δ = 1.05 (t, J = 7.2 Hz, 3H), δ = 1.18 (m, 2H), δ = 1.31 (m, 2H), δ = 2.41 (q, J = 7.2 Hz, 2H), δ = 2.58 (m, 4H), δ = 3.34 (m, 4H), δ = 3.82 (m, 1H), δ = 7.56 (d, J = 7.4 Hz, 1H), δ = 7.89 (d, J = 13.5 Hz, 1H), δ = 8.65 (s, 1H) , δ = 15.16 (s, 1H)

(2) : δ = 1.06 (t, J = 7.2 Hz, 3H), δ = 1.12 (s, 2H), δ = 1.31 (m, 2H), δ = 2.67 (s, 4H), δ = 3.35 (s, 4H), δ = 3.79 (m, 1H), δ = 7.53 (d, J = 5 Hz, 1H), δ = 7.89 (d, J = 13.5 Hz, 1H), δ = 8.67 (s, 1H), δ = 8.81 (s, 1H)

(3) : δ = 1.05 (t, J = 7.2 Hz, 6H), δ = 1.13 (m, 2H), δ = 1.19 (m, 2H), δ = 1.24 (m, 2H), δ = 1.33 (m, 4H), δ = 3.33 (m, 8H), δ = 3.82 (m, 2H), δ = 5.92 (s, 2.7H), δ = 6.56 (d, J = 8.7 Hz, 3.4H), δ = 6.99 (s, 1.8H), δ = 7.54 (d, J = 7.2 Hz, 1H), δ = 7.56 (d, J = 7.2 Hz, 1H), δ = 7.61 (d, J = 8.5 Hz, 3H), δ = 7.88 (d, J = 13.5 Hz, 1H), δ = 7.91 (d, J = 13.5 Hz, 1H), δ = 8.47 (d, J = 4.5 Hz, 3H), 8.67 (s, 1H), δ = 8.87 (s, 1H), δ = 11.15 (s, 1H), δ = 15.16 (s, 1H)

^{19}F NMR (400 MHz, DMSO-d_6)
Enrofloxacin : δ = -123.7 ppm

(2) : δ = -123.7 ppm (2F), δ = -124.7 ppm (1F)

(3) : δ = -123.7 ppm (1F), δ = -124.6 ppm (1F)

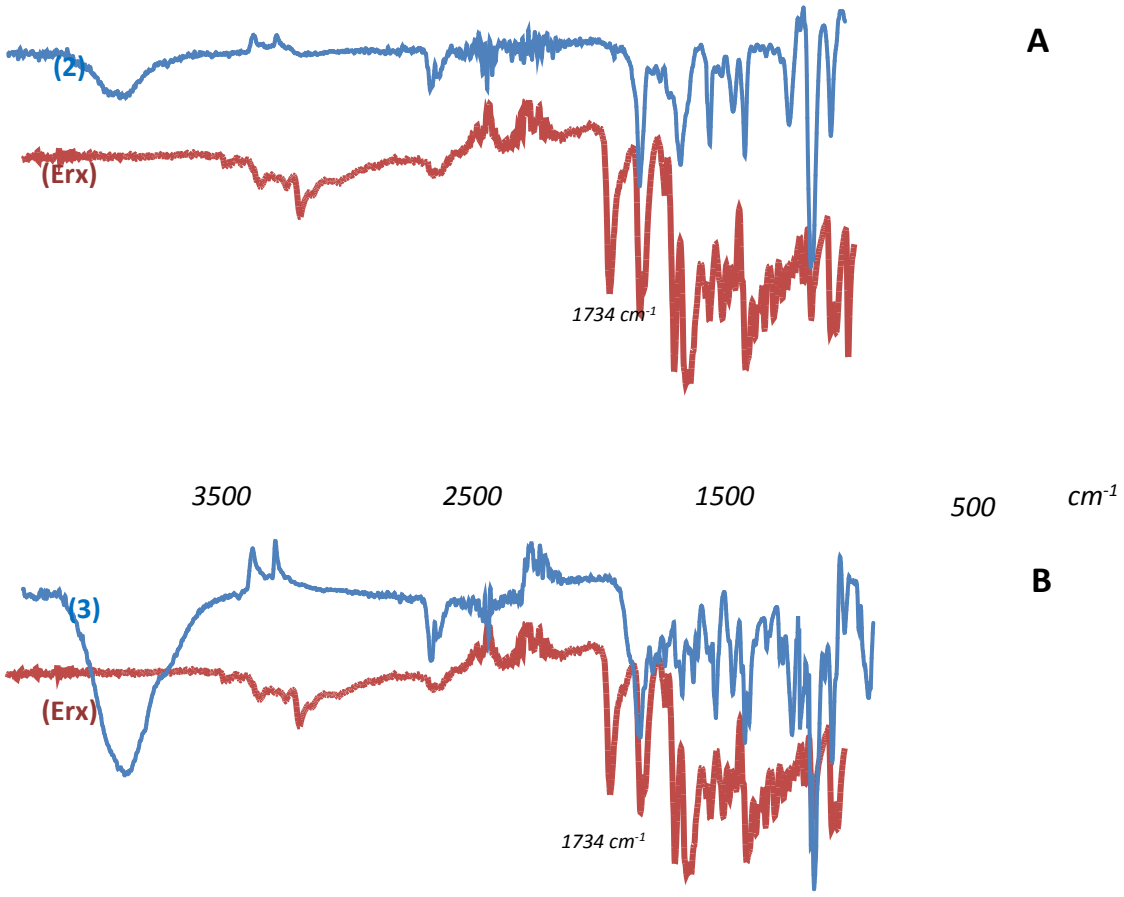

Figure SI-7: IR spectra of Enrofloxacin **(Erx)**, **(2)** and **(3)** in a solid state, (A) comparison of **(2)** with the ligand Erx ; (B) comparison of **(3)** with **Erx**.