Electronic Supporting Material

Coordination complexes of zinc and manganese based on pyridine-2,5-dicarboxylic acid *N*-oxide: DFT studies and antiproliferative activities consideration

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Contents

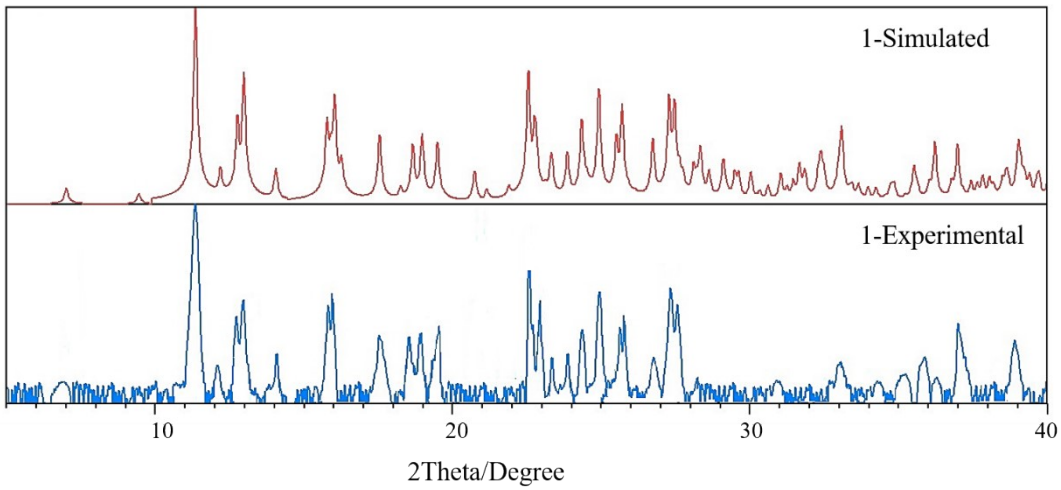


Fig. S1. XRD pattern of **1** (simulated and experimental).

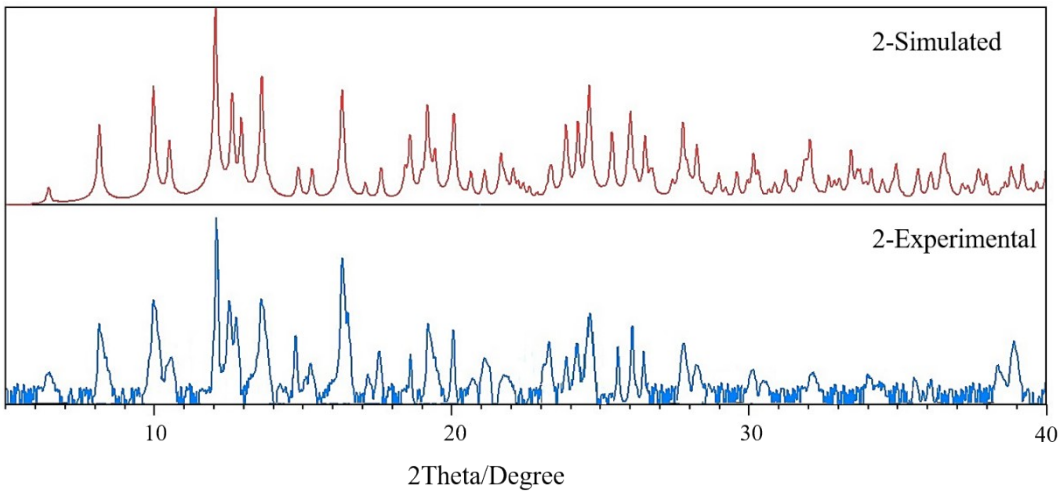


Fig. S2. XRD pattern of **2** (simulated and experimental).

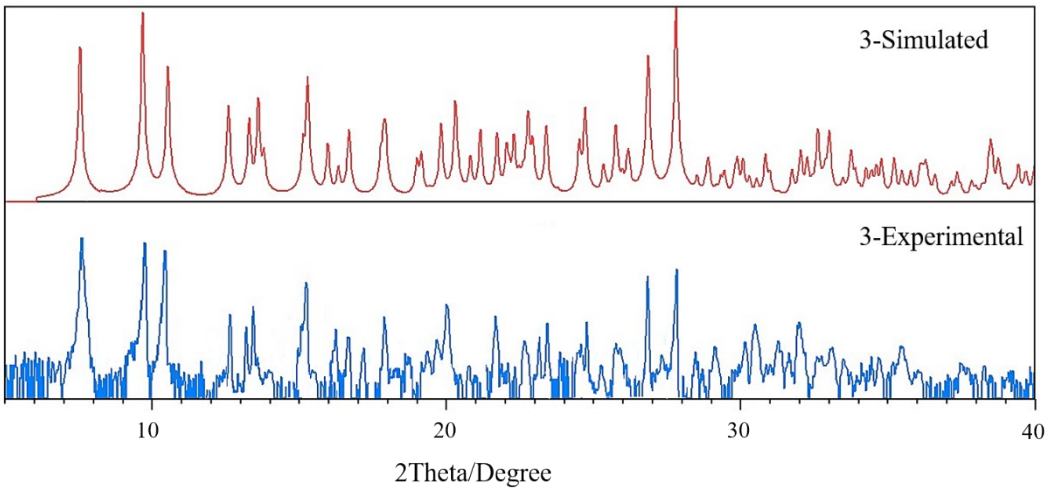


Fig. S3. XRD pattern of **3** (simulated and experimental).

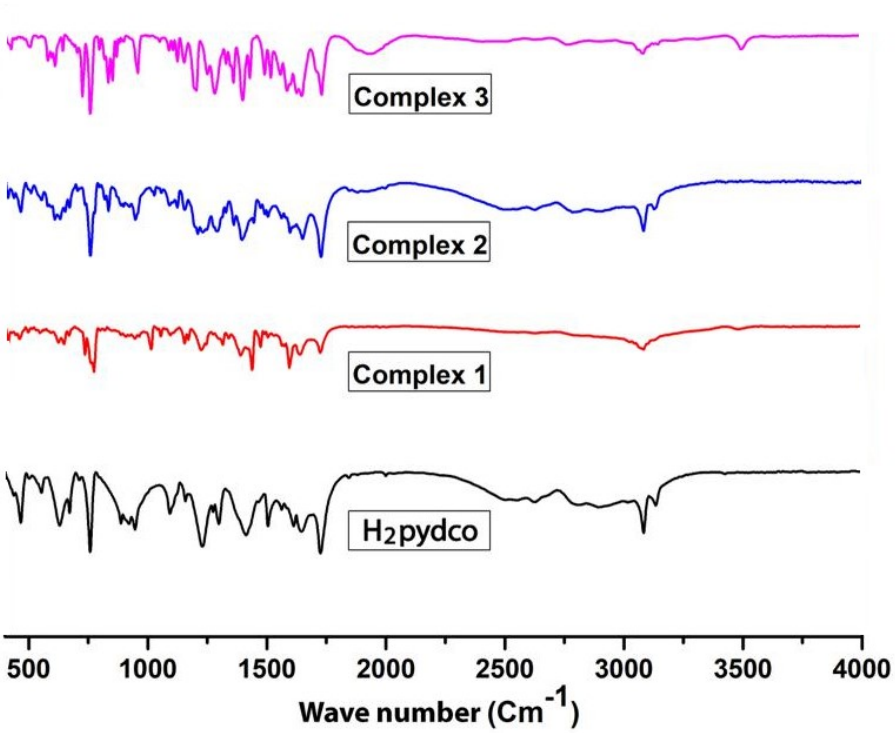


Fig. S4. FTIR spectra of H_2pydco, **1**, **2** and **3**.

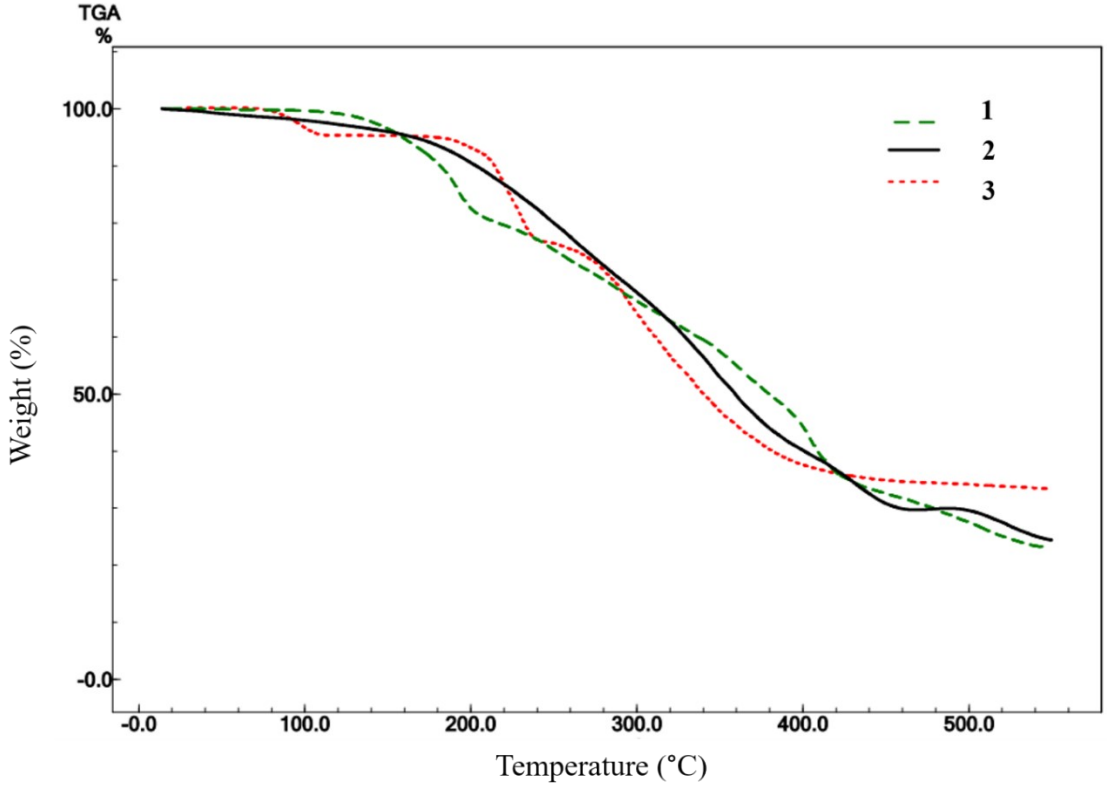
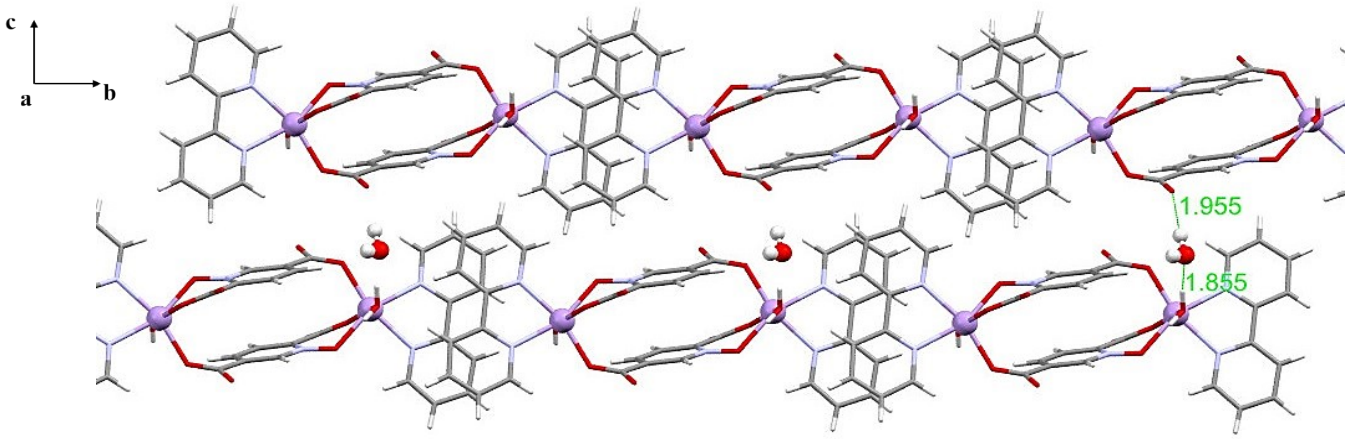


Fig. S5. TGA curves of **1**, **2** and **3**.


c
a
b
1.955
1.855

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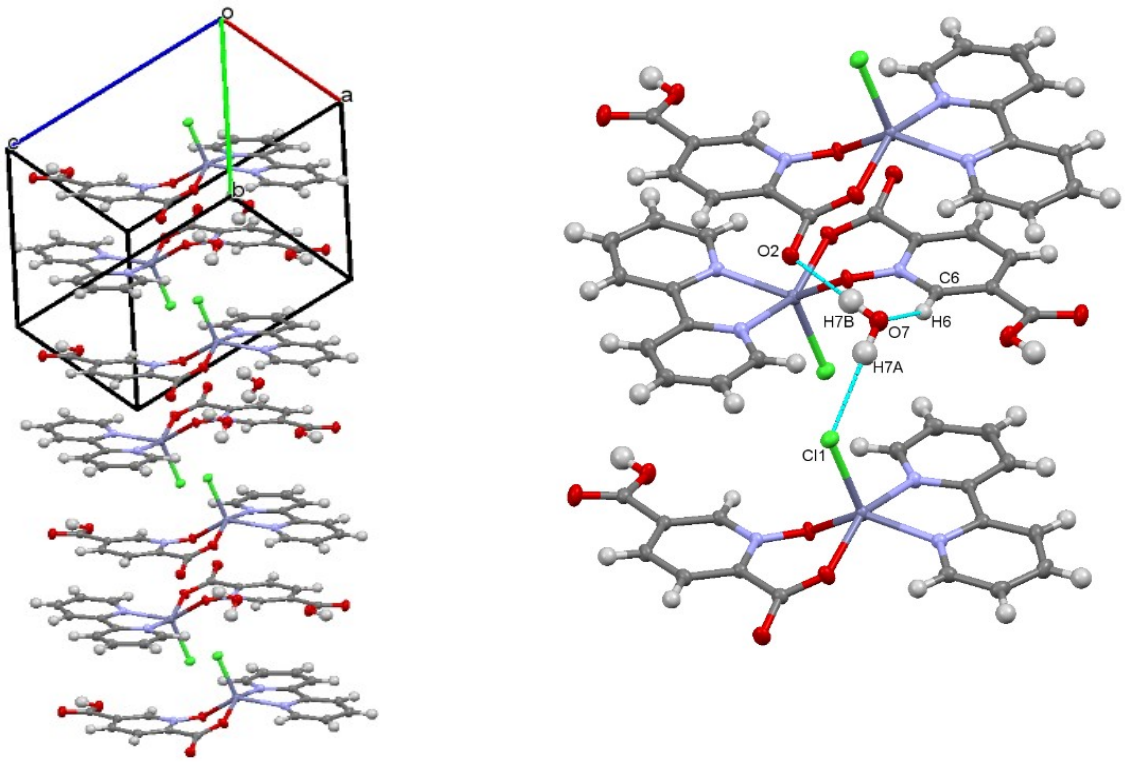


Fig. S7. Representation of the 1D linear chain along the *b* axis in **3**.

Table S1. Selected bond lengths (Å) and angles (°) for **1-3**.

1			
Mn1–O3	2.147(3)	O5–Mn1–O6	92.51(11)
Mn1–O1	2.126(3)	O5–Mn1–N1	91.37(11)
Mn1–O6	2.160(3)	O5–Mn1–N2	163.70(11)
Mn1–O5	2.141(3)	O1–Mn1–N2	95.52(12)
Mn1–N1	2.250(3)	N1–Mn1–N2	72.34(12)
Mn1–N2	2.272(3)	O1–Mn1–O3	78.26(11)
O1–Mn1–O5	89.12(12)	O3–Mn1–N1	159.19(12)
O1–Mn1–N1	104.64(11)	O1–Mn1–O6	159.05(11)
O3–Mn1–N2	86.90(11)	O6–Mn1–N2	88.73(11)
O5–Mn1–O3	109.36(11)	O6–Mn1–N1	96.21(11)
O3–Mn1–O6	81.51(10)	O5–Mn1–O6	92.51(11)
2			
Zn1–O1	2.0706(18)	N4–Zn1–O6	97.09(8)
Zn1–N3	2.101(2)	O1–Zn1–O3	82.63(7)
Zn1–N4	2.108(2)	N3–Zn1–O3	91.56(8)
Zn1–O6	2.1152(19)	N4–Zn1–O3	97.33(8)
Zn1–O3	2.120(2)	O6–Zn1–O3	88.81(7)
Zn1–O8	2.129(2)	O1–Zn1–O8	88.58(7)
O1–Zn1–N3	90.99(8)	N3–Zn1–O8	97.88(8)
O1–Zn1–N4	169.20(8)	N4–Zn1–O8	93.04(8)
N3–Zn1–N4	78.21(9)	O6–Zn1–O8	82.50(7)
O1–Zn1–O6	93.71(7)	O3–Zn1–O8	167.22(7)
N3–Zn1–O6	175.29(8)	N4–Zn1–O6	97.09(8)
3			
Zn1–O1	2.0242(10)	O3–Zn1–N3	87.54(4)
Zn1–N2	2.0951(12)	O1–Zn1–Cl1	101.86(3)
Zn1–Cl1	2.2739(4)	N2–Zn1–Cl1	115.44(3)
Zn1–O3	2.0251(10)	O1–Zn1–N2	89.51(4)
Zn1–N3	2.1186(12)	O1–Zn1–N3	153.79(5)
O1–Zn1–O3	86.15(4)	N2–Zn1–N3	77.38(5)
O3–Zn1–N2	135.47(4)	O3–Zn1–Cl1	108.81(3)

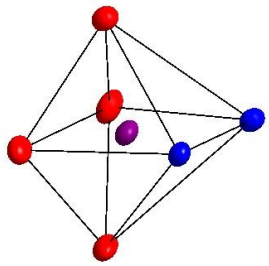
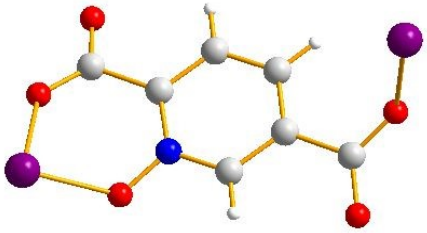
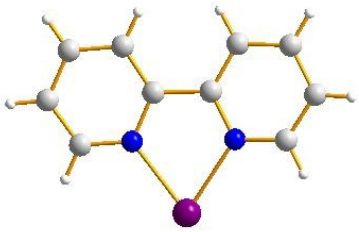
Complex	Coordination mode of metallic centre	Coordination mode of the main ligand	Coordination mode of auxiliary ligand
1			

Table S2. Selected Hydrogen bond geometry, lengths (Å) and angles (°) for **1-3**.

D–H···A	D–H	H···A	D···A	D–H···A
1				
O6–H6A···O7	0.87	1.85	2.714(4)	168.8
O6–H6B···O2	0.87	1.87	2.742(4)	175.9
C4–H4···O6	0.95	2.55	3.399(5)	148.4
C7–H7···O7	0.95	2.55	3.269(5)	132.4
C10–H10···O3	0.95	2.50	3.102(5)	121.3
C16–H16···O2	0.95	2.56	3.377(5)	143.9
O7–H7A···O4	0.87	1.95	2.824(4)	177.3
O7–H7B···O4	0.87	2.04	2.870(4)	160.2
2				
O4–H4A···O2	0.87	1.69	2.556(3)	176.5
O9–H9···O6	0.87	1.77	2.631(3)	172.1
C3–H3···O5	0.95	2.32	3.084(3)	136.7
C10–H10···O10	0.95	2.51	3.330(3)	145.2
C23–H23···O7	0.95	2.42	3.283(4)	150.9
3				
O4-H4A···O6	0.87	1.67	2.5239(16)	167.0
C6-H6···O7	0.95	2.38	3.2645(18)	155.1
C11-H11···O5	0.95	2.49	3.3508(18)	151.4
O6-H6A···O7	0.87	1.82	2.6886(17)	177.8
O6-H6B···O5	0.87	1.97	2.8283(16)	169.5
O7-H7A···Cl1	0.87	2.34	3.2103(12)	177.2
O7-H7B···O2	0.87	1.89	2.7552(16)	178.4

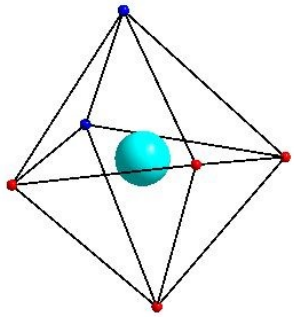
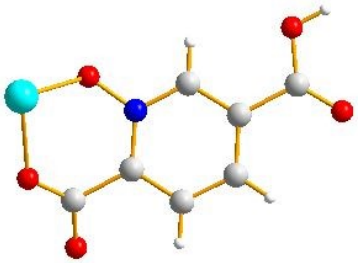
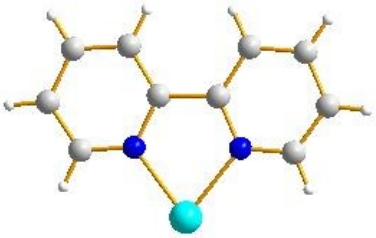
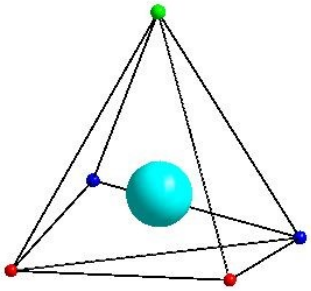
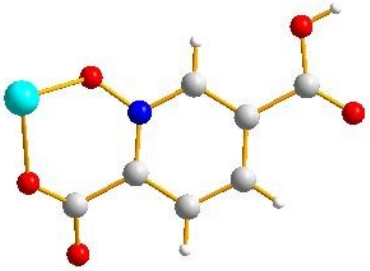
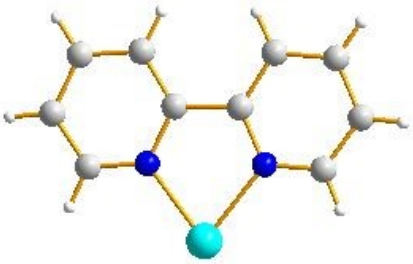
2			
3			

Table S3. Coordination modes of the metallic centres and organic ligands in **1**-**3**.