Supplementary information

Table S1. Comparison of crystal parameters of compound **2** with the already reported compound

| Crystal Parametres	**2**	**CCDC 1852819**
Emprical formula	$C_5H_6Cl_2ZnN_2$	$C_5H_6Cl_2N_2Zn$
Formula weight	230.39	230.39
Temperature (K)	100.0	103.0
Crystal system	Monoclinic	Monoclinic
Space group	*Cc*	*Cc*
a/Å	13.6324(10)	13.6431(10)
b/Å	7.5986(6)	7.6070(3)
c/Å	8.3812(6)	8.3818(8)
α °	90	90
β°	116.926(2)	116.946(10)
γ °	90	90
Volume (Å^3)	774.07(10)	775.45(10)
Z	4	4
Calculated density (g/cm^3)	1.977	1.973
Absorption coefficient (mm^{-1})	10.113	Not available
F(000)	456.0	456.0
Crystal size (mm^3)	0.32× 0.23 × 0.17	0.10×0.05×0.03
Index ranges	-16 ≤ h ≤ 15,-9 ≤ k ≤9, -9 ≤ l ≤ 9	-17 ≤ h ≤ 15,-9 ≤ k ≤9, -10 ≤ l ≤ 10
Reflections collected	4757	1542
Unique data(R_{int})	1330	1541
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1330/2/93	Not available
Goodness-of-fit on F^2	1.072	1.115
Final *R*indices[$I>2\sigma$ (*I*)] *R*1/ *wR*2	0.0282/0.0729	0.0167/0.0453
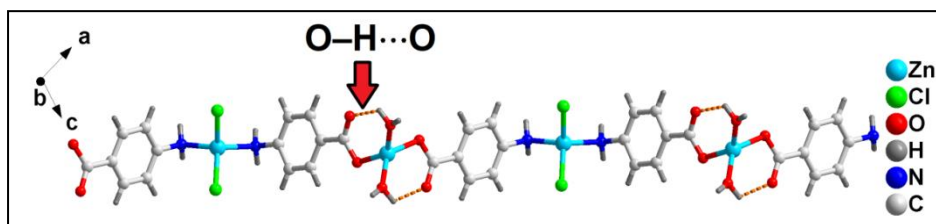
Figure S1 1D polymeric chain of compound **1** assisted by intra-molecular O–H···O hydrogen bonding interactions.
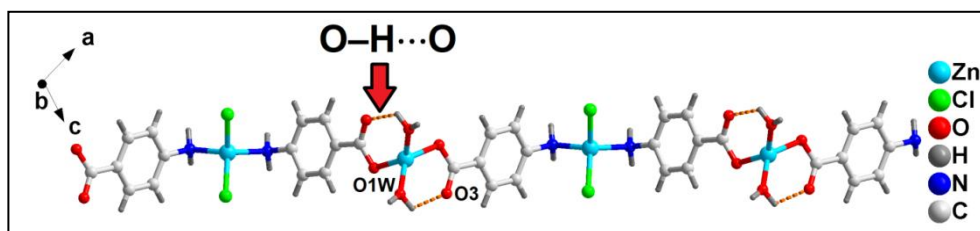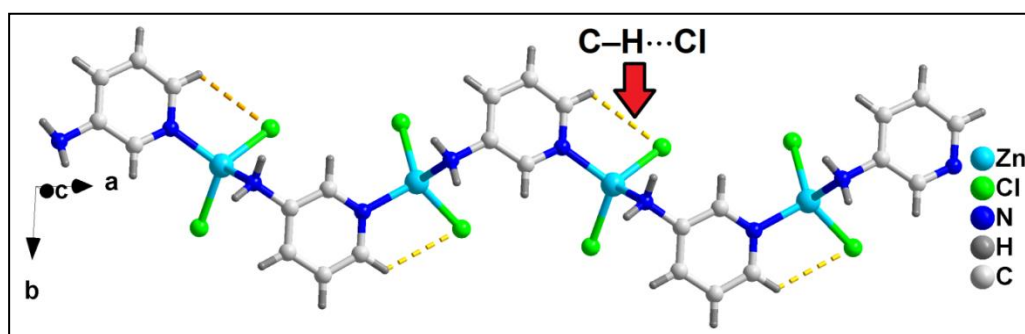
Figure S2 1D polymeric chain of compound **2** stabilised by C–H···Cl hydrogen bonding interactions.
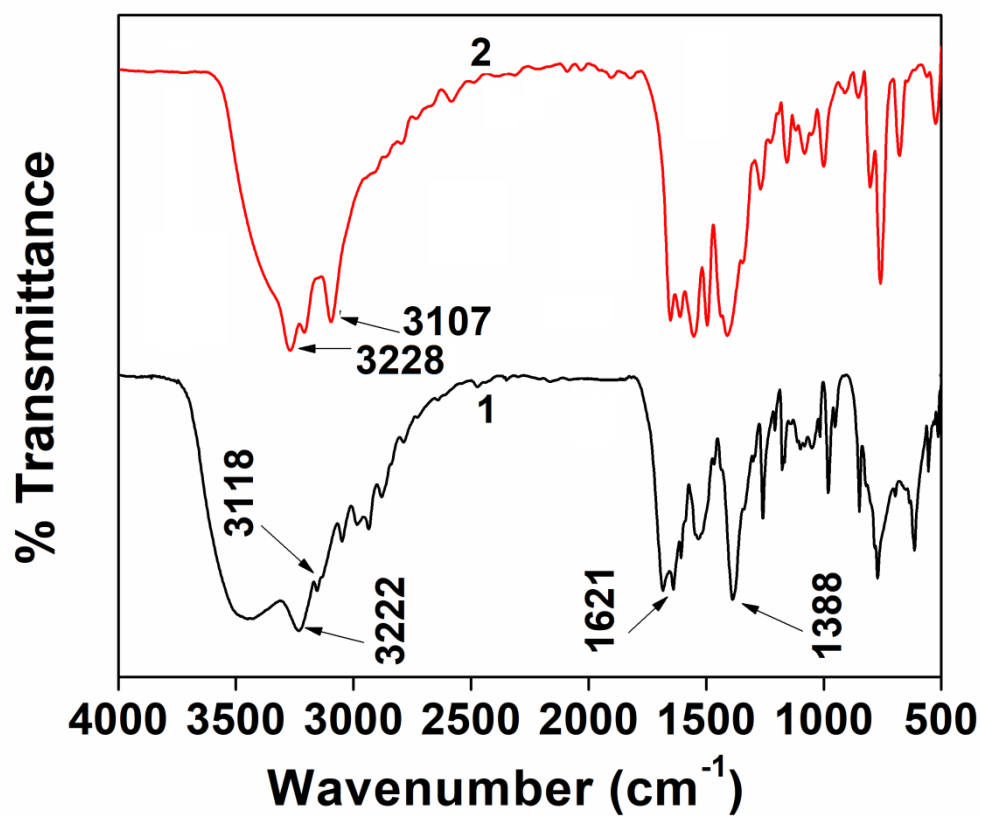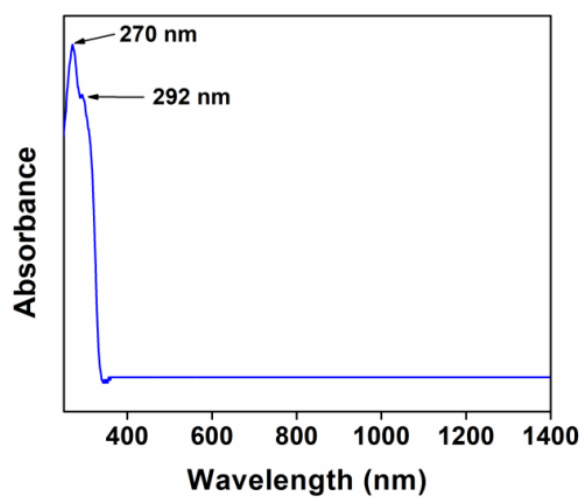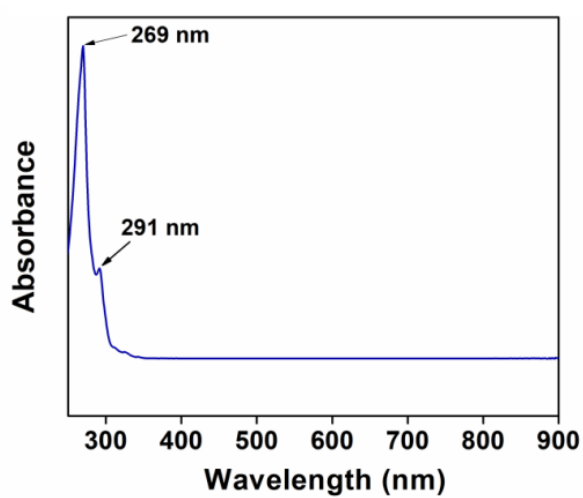

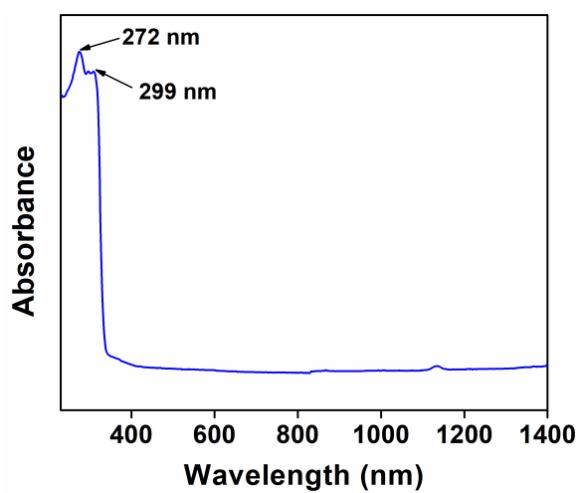**Figure S3** FT-IR spectra of the compounds **1** and **2**.

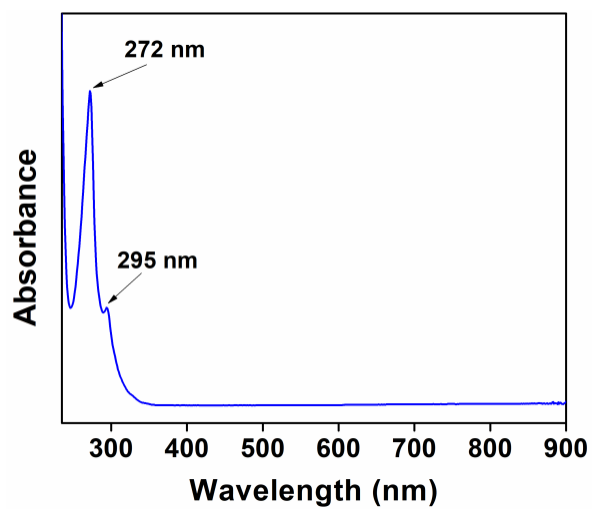(**a**)   (**b**)

Figure S4(**a**) UV-Vis-NIR spectrum of **1**; (**b**) UV-Vis spectrum of **1** in water (10^{-3} M).

(**a**)   (**b**)

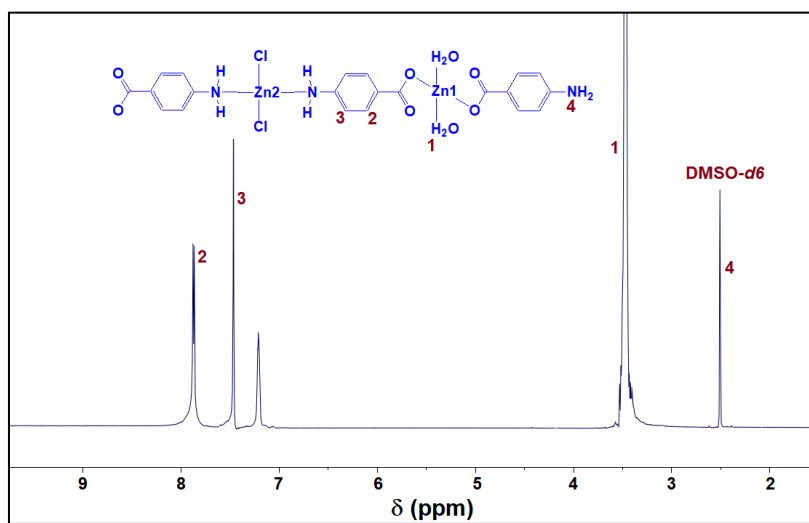**Figure S5**(**a**) UV-Vis-NIR spectrum of **2**; (**b**) UV-Vis spectrum of **2** in water (10^{-3} M).

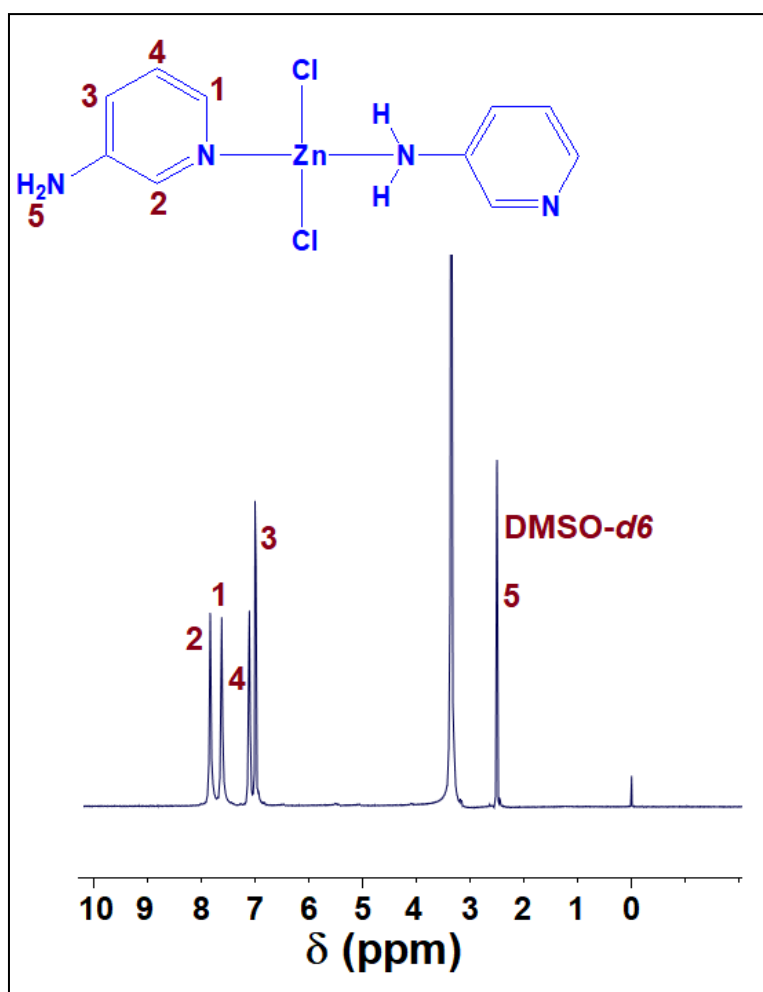**Figure S6** ^{1}H-NMR spectrum of compound **1** in DMSO-*d6*.

Figure S7 ^{1}H-NMR spectrum of compound **2** in DMSO-*d6*.
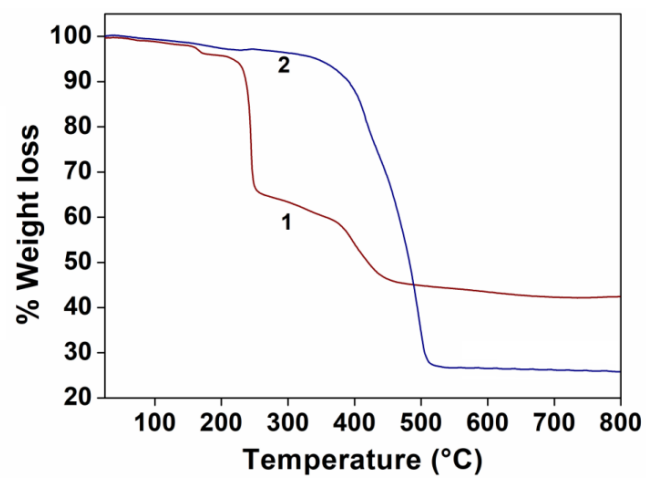

Figure S8 Thermogravimetric curves of the compounds **1** and **2**.

Table S2 IC$_{50}$ values (in μM) of compounds **1**, **2**, ligands and metal salt calculated using dose response curves.

Sl. Nos.	Drug candidates	Cell lines	Nature of cell lines	IC$_{50}$	Error (S.E.)
1.	Cisplatin (Reference)	DL	Malignant cancer	0.61	0.32
2.	Compound **1**	DL	Malignant cancer	5.8	0.42
3.	Compound **2**	DL	Malignant cancer	16.80	0.38
4.	ZnCl$_2$	DL	Malignant cancer	64	0.87
5.	4-AmBz	DL	Malignant cancer	318	2.52
6.	3-AmPy	DL	Malignant cancer	410	3.21
7.	Compound **1**	PBMC	Normal cell	310	2.42
8.	Compound **2**	PBMC	Normal cell	380	2.92
9.	ZnCl$_2$	PBMC	Normal cell	398	3.56
10.	4-AmBz	PBMC	Normal cell	418	3.55
11.	3-AmPy	PBMC	Normal cell	450	4.22