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

Supplementary Information

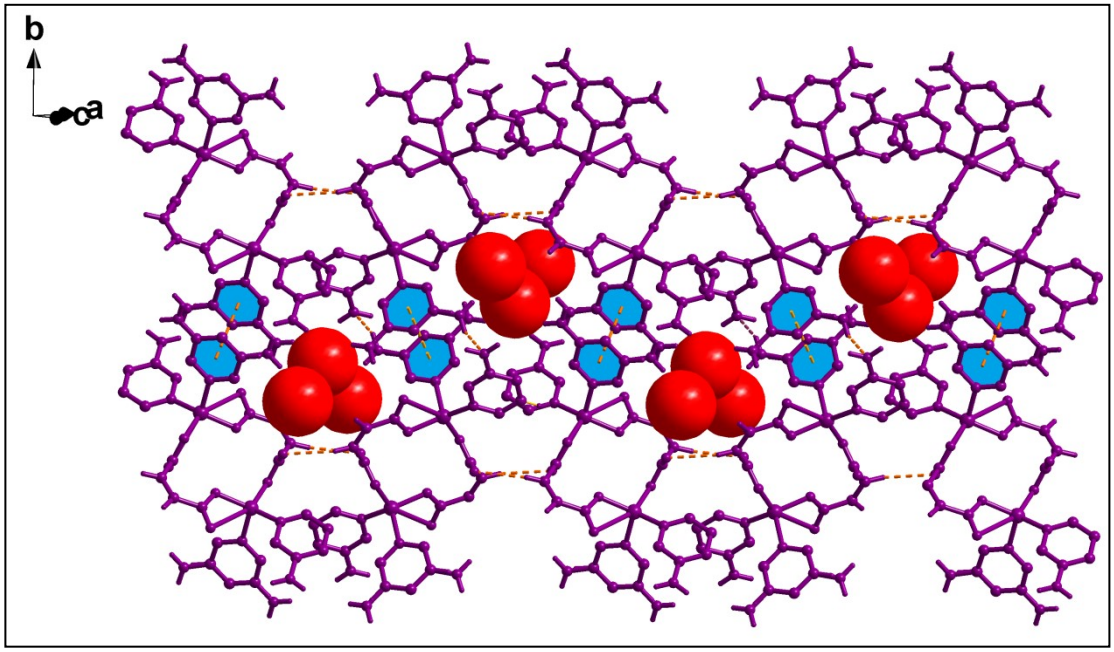

Fig. **S1** Layered assembly of the compound **2** involving the enclathrated V-shaped $(H_2O)_3$ cluster along the *ab* plane.

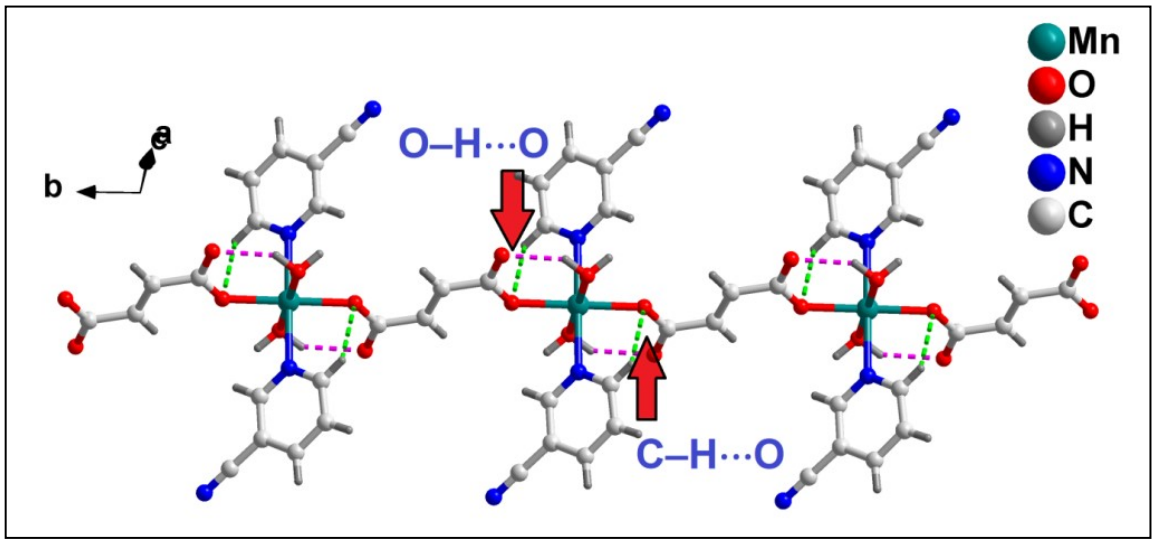

Fig. **S2** 1D polymeric chain of compound **2** stabilized by intra-molecular O–H···O and C–H···O hydrogen bonding interactions.

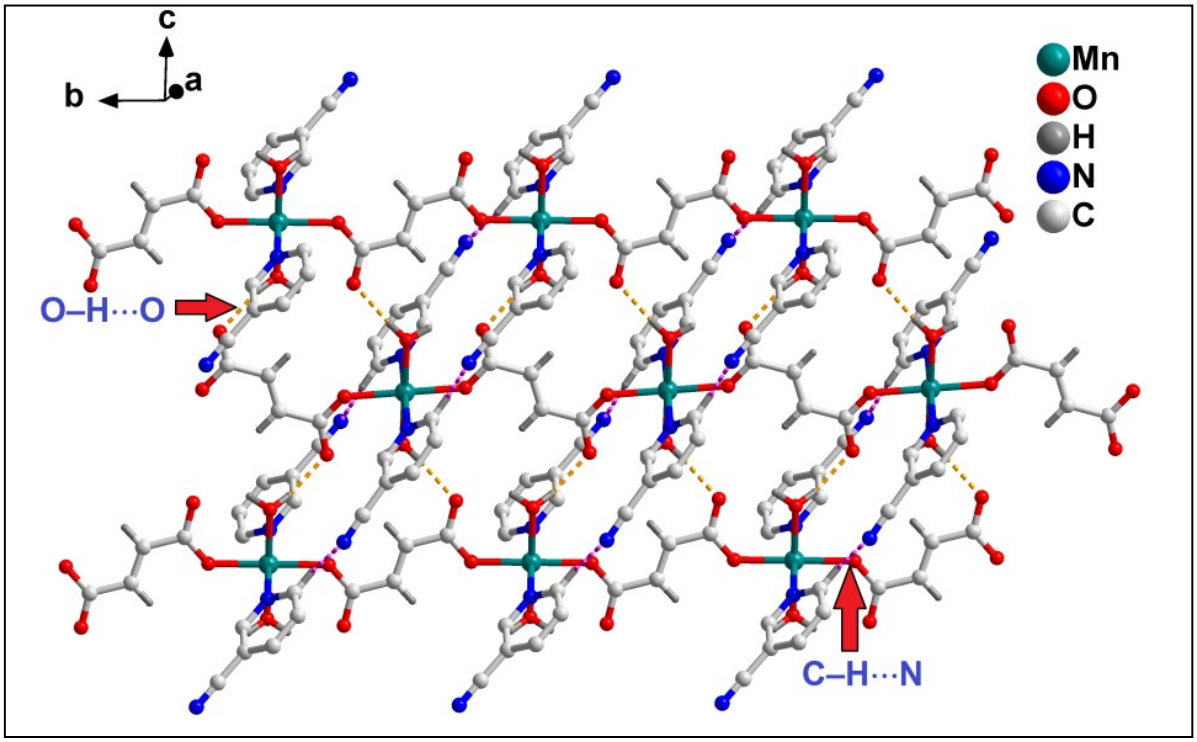

Fig. **S3** Layered assembly of compound **2** along the crystallographic *bc* plane.

Table S1 Selected hydrogen bond distances (Å) and angles (°) for the compounds **1** and **2**.

D–H···A	*d*(D–H)	*d*(D···A)	*d*(H···A)	<(DHA)
1				
N4B–H4BA···O3#1	0.880(4)	3.195(4)	2.419(1)	147.2(2)
C5B–H5B···O3	0.950(3)	3.478(3)	2.755(2)	133.4(3)
O2W–H2W···O1W	1.013(4)	2.791(5)	1.878 (3)	170.4(3)
N4B–H4BB···O2W#2	0.879(1)	2.880(4)	2.103(2)	146.8(2)
N8B–H8BA···N4A#1	0.880(1)	3.019(2)	2.240(7)	147.3(4)
C5–H5···O8	0.950(1)	3.528(1)	2.709(2)	144.7(2)
O1W–H1WB···O8	0.869(2)	2.867(1)	2.019(2)	145.3(2)
2				
O1W–H1WA···O13A	0.875(9)	2.777(1)	2.039(9)	141.1(6)
C16–H16···O11A	0.950(2)	3.275(2)	2.849(1)	108.3(9)
C24–H24···O13A	0.950(1)	3.377(5)	2.486(1)	155.1(1)
O2W–H2WA···O13A	0.875(2)	2.715(3)	1.934(7)	162.3(1)
O1W–H1WB···O23A	0.876(1)	2.778(1)	1.961(4)	161.2(3)
C16–H16···N18	0.950(1)	3.263(2)	2.740(1)	115.4(3)
C26–H26···N28	0.950(1)	3.295(2)	2.746(2)	121.4(1)

#1 1/2-X, 1/2-Y, 1-Z; #2 -1/2+X, -1/2+Y, +Z

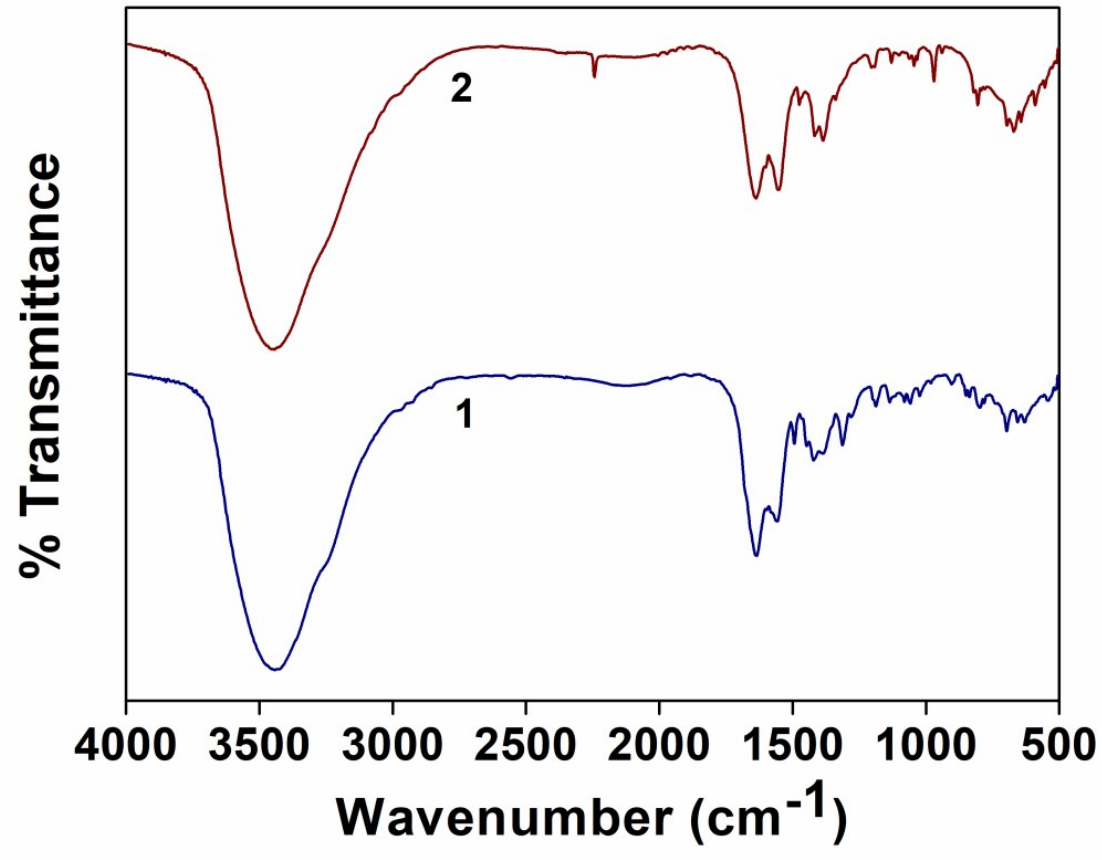

Fig. **S4** FT-IR spectra of the compounds **1** and **2**.

3.3.2 Electronic spectroscopy

The electronic spectra of the compounds **1** and **2** have been recorded in solid as well as in aqueous state (Figs. S5 and S6). The electronic spectra of the diamagnetic Zn(II) dimeric complex do not show any absorption bands in the visible regions.[1] The absorption bands at 234 and 268 nm in the UV-Vis-NIR spectrum (Fig. S5a) of compound **1** can be attributed to the $\pi \rightarrow \pi^*$ transition of the aromatic ligands.[2] These absorption peaks are obtained at 231 and 267 nm in the aqueous phase UV-Vis spectrum (Fig. S5b).[2]

The electronic spectra of compound **2** also do not exhibit any absorption bands in the visible region, as Mn(II) centre (d^5 system) has all the electronic transitions from the $^6A_{1g}$ ground state doubly forbidden.[3,4] The peaks at 230 and 271 nm in the solid state UV-Vis-NIR spectrum

(Fig. S6a) can be assigned as the π→π* transition of the aromatic ligands.[5] In the aqueous state UV-Vis spectrum (Fig. S6b), these absorption peaks were obtained at 226 and 265 nm respectively.[5]

The observed similarities in the absorption peaks of compounds **1** and **2** in both the phases suggest that the compounds do not undergo any structural distortion in the aqueous phase.[6]

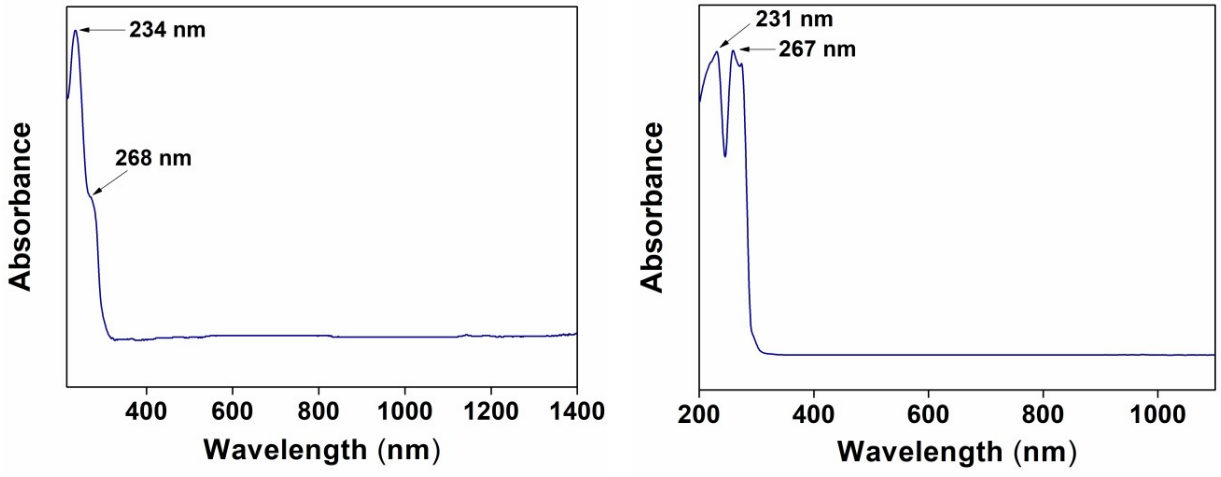

Fig. **S5**(**a**) UV-Vis-NIR spectrum of **1** (**b**) UV-Vis spectrum of **1** in water.

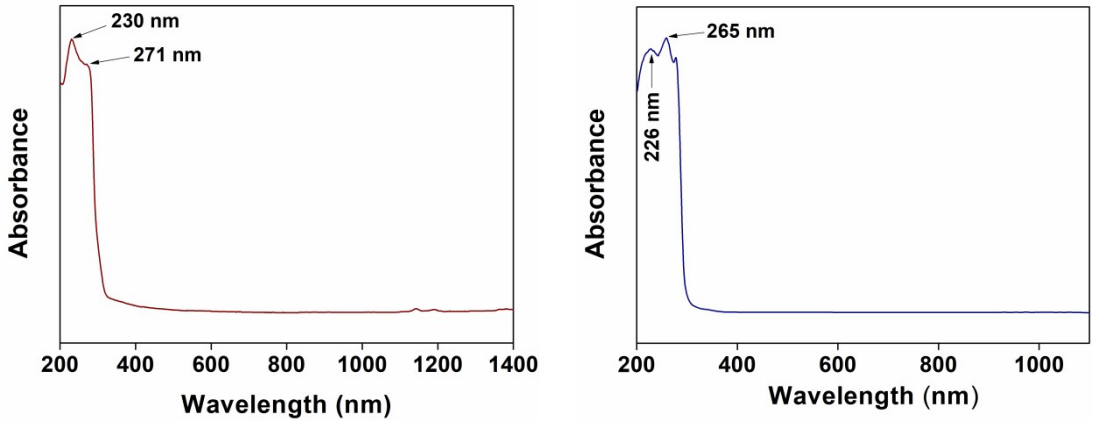

Fig. **S6**(**a**) UV-Vis-NIR spectrum of **2** (**b**) UV-Vis spectrum of **2** in water.

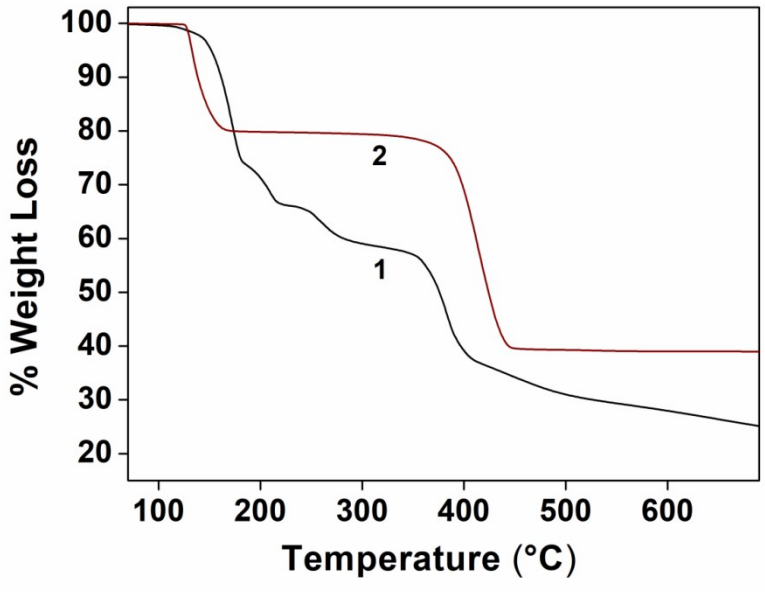

Fig. **S7** Thermogravimetric curves of the compounds **1** and **2**.

Table S2 IC_{50} values (μM) of compounds **1** and **2** in normal (PBMC) and cancerous cells (DL) after 24 hours of treatment.

Sl. Nos.	Drug candidates	Cell lines	Nature of cell lines	IC_{50}	Error (S.E.)
1.	Cisplatin (Reference)	DL	Malignant cancer	0.19	0.03
2.	Compound **1**	DL	Malignant cancer	5.90	0.03
3.	Compound **2**	DL	Malignant cancer	23.75	0.14
4.	Compound **1**	PBMC	Normal cell	229.72	0.077
5.	Compound **2**	PBMC	Normal cell	289.68	0.090

Table S3 Intermolecular interactions between receptors and compounds. The reference ligands were used from PDB entry file of respective receptor. As per binding energy calculation algorithm in MVD software, the binding scores are represented as arbitrary unit. Lower the score better is the affinity between compounds and receptors.

Sl. Nos.	Receptors	Ligands	No. of H-bond	Interactive amino acids	Binding score
1	BCL-2 (2O22)	Reference ligand	4	Gly142, Arg104, Thr93	-157
		Compound-1	4	Tyr199, Tyr105, Asp100	-146
		Compound-2	1	Ala97	-111
2	BCL-XL (2YXJ)	Reference ligand	4	Gly138, Glu129	-145
		Compound-1	2	Val126, Phe105	-132
		Compound-2	1	Arg139	-108

3	MCL-1 (5VKC)	Reference ligand	4	Arg263, Leu267	-176
		Compound-1	3	Ala227, Thr266, Arg263	-154
		Compound-2	1	Arg263	-139

Supplementary References

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