Supplementary Information

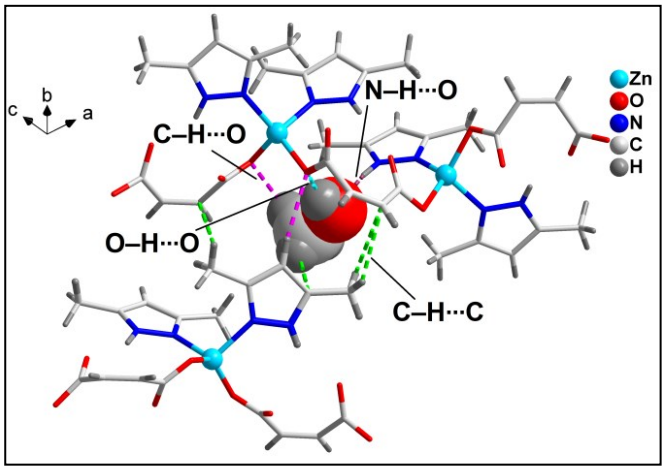
Table S1 Selected bond lengths (Å) and bond angles (°) of Zn(II) centers in **1** and **2**.

Bond distances of **1** (in Å)		Bond angles of **1** (in Degree)	
Zn1-O1A	1.959(5)	O1A-Zn1-O8B	100.95(19)
Zn1-O8B	2.003(4)	O1A-Zn1-N11	131.0(2)
Zn1-N11	2.010(5)	O1A-Zn1-N11'	106.0(2)
Zn1-N11'	2.030(5)	O8B-Zn1-N11'	101.5(2)
Zn2-O1B	1.947(5)	N11-Zn1-N11'	103.0(2)
Zn2-O8C	1.966(5)	O1B-Zn2-O8C	136.2(2)
Zn2-N21	2.025(6)	O1B-Zn2-N21	99.2(2)
Zn2-N21'	2.040(5)	O8C-Zn2-N21	107.9(2)
Zn3-O1C	1.974(5)	O1B-Zn2-N21'	103.9(2)
Zn3-O8A#1	1.985(5)	O8C-Zn2-N21'	101.3(2)
Zn3-N31'	2.017(5)	N21-Zn2-N21'	105.4(2)
Zn3-N31	2.037(5)	O1C-Zn3-O8A#1	121.5(2)
		O1C-Zn3-N31'	108.5(2)
		O8A#1-Zn3-N31'	100.4(2)
		O1C-Zn3-N31	102.5(2)
		O8A#1-Zn3-N31	119.8(2)
		N31'-Zn3-N31	102.2(2)

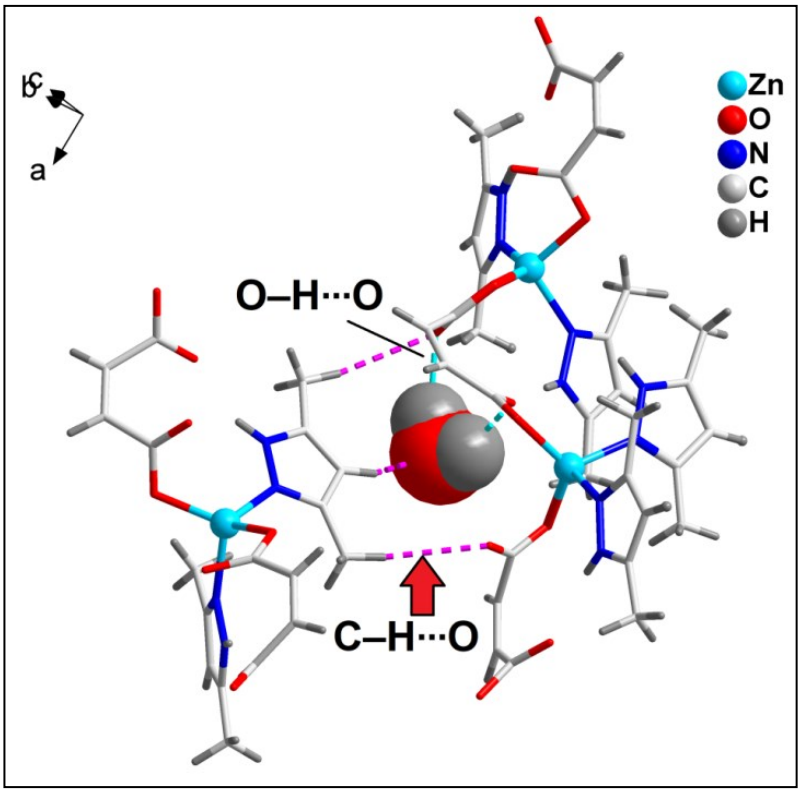
#1 x-1, y, z+1

Bond distances of **2** (in Å)		Bond angles of **2** (in Degree)	
Zn-O3	2.051(13)	O3-Zn-O5#1	178.9(6)
Zn-O5#1	2.099(12)	O3-Zn-N2	93.3(5)
Zn-N2	2.149(11)	O5#1-Zn-N2	87.6(5)
Zn-N1	2.151(11)	O3-Zn-N1	88.1(5)
Zn-O2	2.159(8)	O5#1-Zn-N1	91.0(5)
Zn-O1	2.168(8)	N2-Zn-N1	178.6(7)
		O3-Zn-O2	90.2(4)
		O5#1-Zn-O2	89.2(4)
		N2-Zn-O2	91.5(4)
		N1-Zn-O2	88.8(3)
		O3-Zn-O1	90.7(4)
		O5#1-Zn-O1	89.9(4)
		N2-Zn-O1	88.8(3)
		N1-Zn-O1	90.8(4)
		O2-Zn-O1	179.1(6)

#1 x, y+1, z



(**a**)



(**b**)

Fig. **S1**(**a**) Enclathration of guest MeOH in the supramolecular host of compound **1**; (**b**) Enclathration of guest water in the supramolecular host of compound **1**.

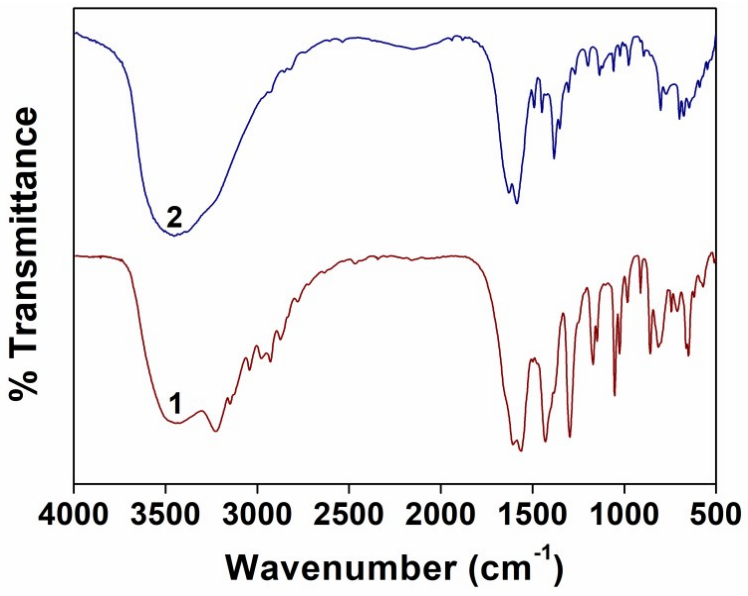


Fig. **S2** FT-IR spectra of the compounds **1** and **2**.

3.4.2 Electronic spectroscopy

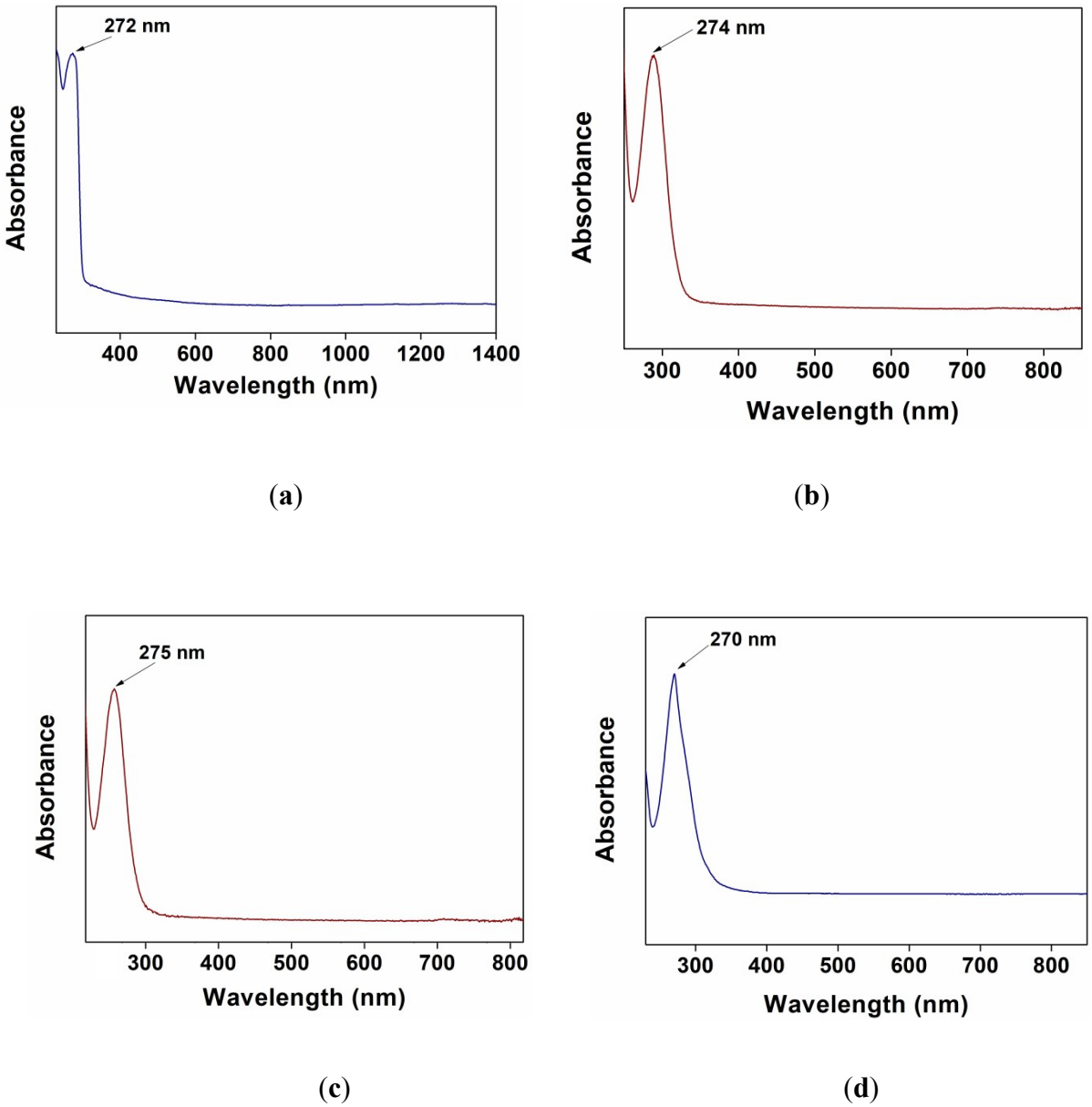


Fig. **S3**(**a**) UV-Vis-NIR spectrum of **1**; (**b**) UV-Vis spectrum of **1** in water; (**c**) UV-Vis spectrum of **1** in DMSO; (**d**) UV-Vis spectrum of **1** in methanol.

The electronic spectra of the compounds **1** and **2** in solid phase as well as in solution phase (water, DMSO and methanol) are shown in Fig. S3 and Fig. S4, respectively. The diamagnetic Zn(II) polymers do not exhibit absorption bands in the visible region.[1] Similar electronic spectra was also reported for Zn(II) complex of schiff base ligand 2-((1H-Benzo [*d*]imidazole-4ylimmino) methyl phenol.[2] For compound **1**, the absorption peaks at 272, 274, 275 and 270 nm in UV-Vis-NIR (Fig. S3a), in aqueous medium (Fig. S3b), in DMSO (Fig. S3c) and in methanol (Fig. S3d) respectively can be attributed to the $\pi \rightarrow \pi^*$ transitions of

aromatic ligands.[3] For compound **2**, the characteristic absorption bands ranging from 271-275 nm in the solid state UV-Vis-NIR (Fig. S4a), in aqueous phase (Fig. S4b), in DMSO (Fig. S4c) and in methanol (Fig. S4d) respectively can be assigned to the $\pi \rightarrow \pi^*$ transitions of aromatic ligands.[4]

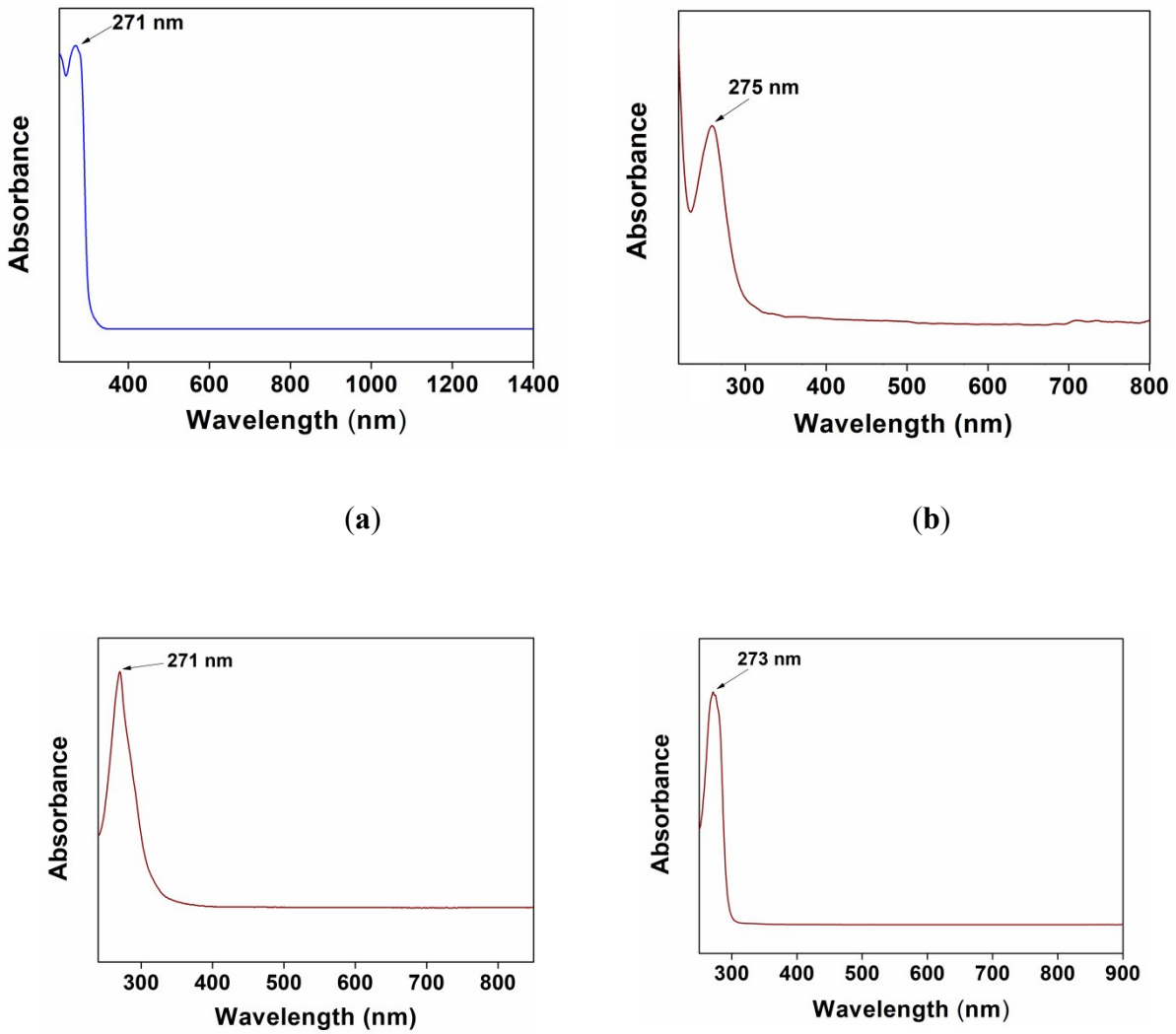


Fig. **S4**(**a**) UV-Vis-NIR spectrum of **2**; (**b**) UV-Vis spectrum of **2** in water; (**c**) UV-Vis spectrum of **2** in DMSO; (**d**) UV-Vis spectrum of **2** in methanol.

From the electronic spectra of **1** and **2** in both the solid and aqueous state, it can be observed that the electronic spectra in aqueous phase do not show marked differences from that of the respective solid-state spectra. So, it may be assumed that bonding modes as well as the geometries of **1** and **2** does not change in the solution phase.[5]

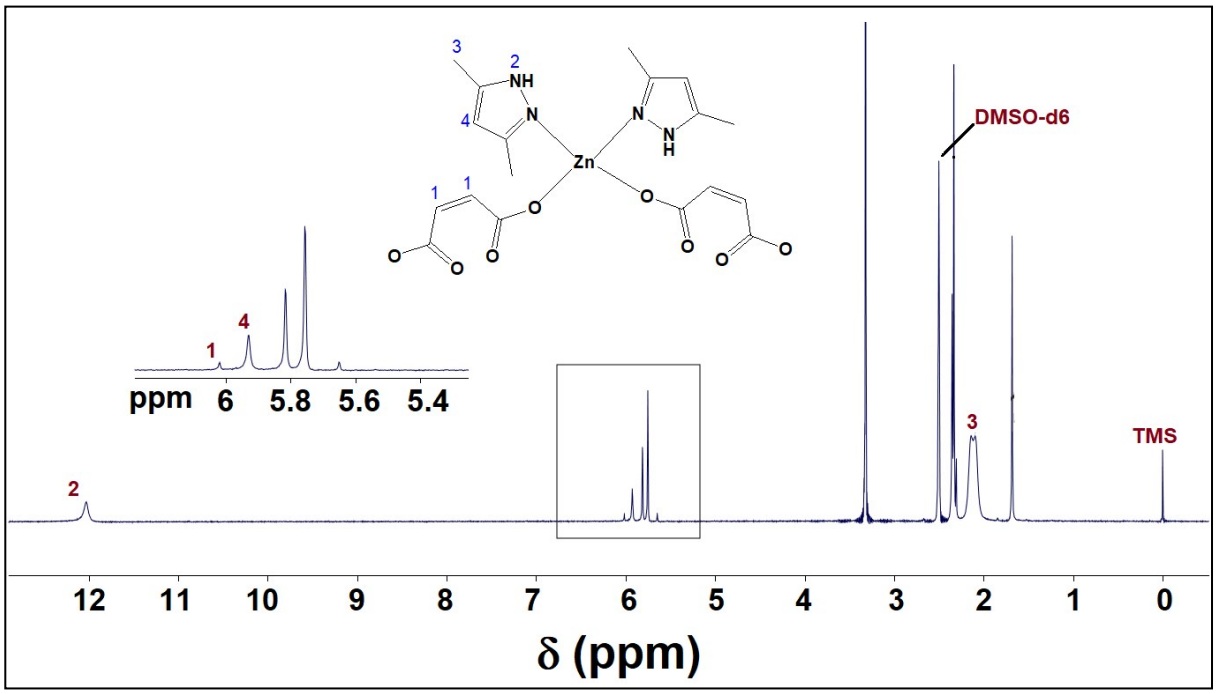


Fig. **S5** [1]H-NMR spectrum of compound **1** in DMSO-d6.

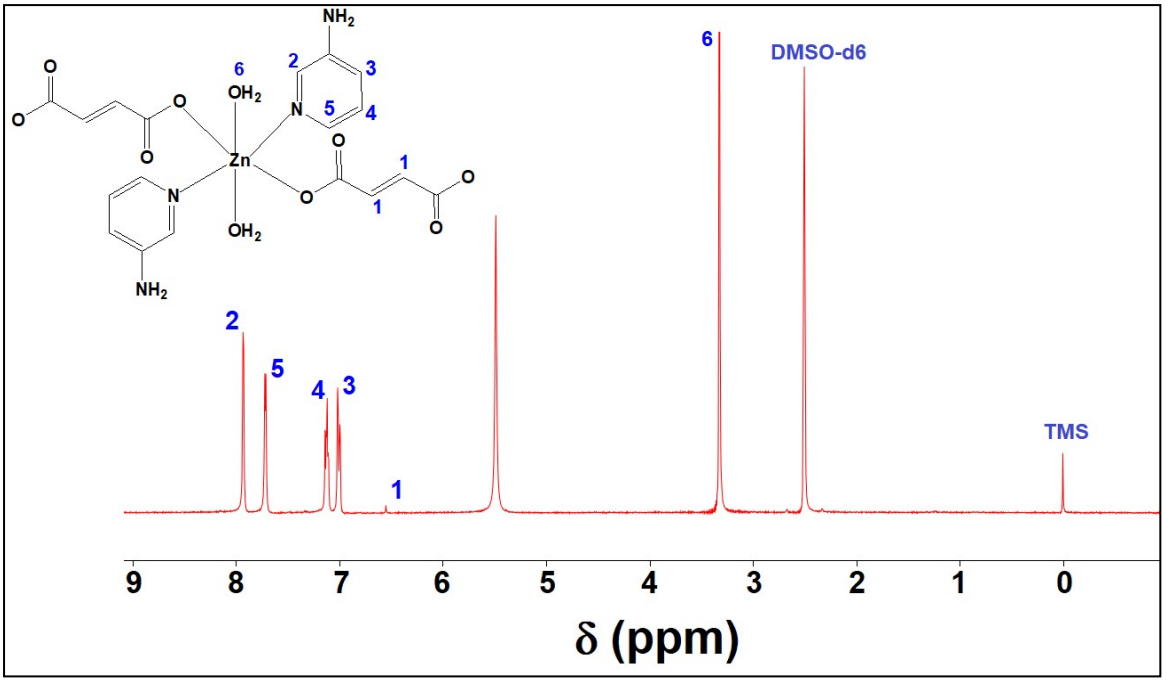


Fig. **S6** [1]H-NMR spectrum of compound **2** in DMSO-d6.

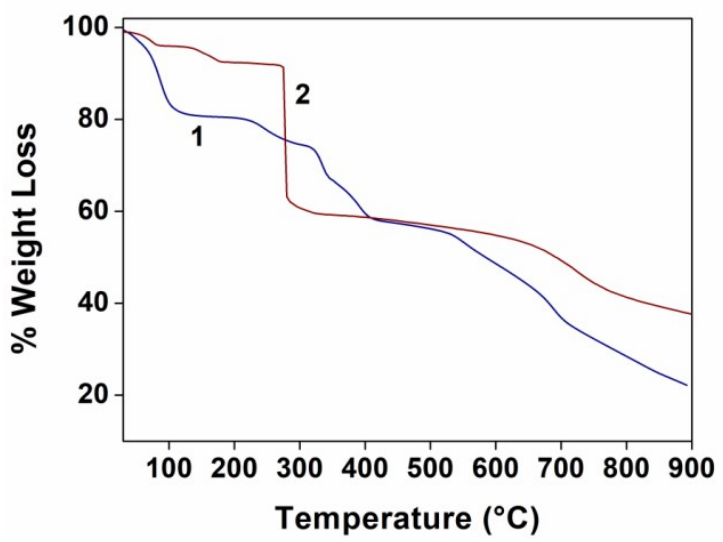


Fig. **S7** Thermogravimetric curves for the compounds **1** and **2**.

Table S2 Cell cytotoxicity of *male*, *Hdmpz*, *fum*, *3-AMpy* and $ZnCl_2$ in DL cells. Data represents % cell death as compared to respective untreated control.

Dose (μM)	% Cytotoxicity				
	male	*Hdmpz*	*fum*	*3-AMpy*	$ZnCl_2$
0.01	0	0	0	0	0
0.1	0	0	0	0	0
0.5	0	0	0	0	3
1	0	0	0	0	4
5	0	0	0	0	6
10	0	0	2	0	8
20	0	0	2	2	10
40	2	2	3	2	12
60	2	3	4	3	12
80	3	3	4	4	14
100	4	4	5	4	14
IC_{50}	**IC_{50}** could not be calculated due to very low cytotoxicity				

Table S3 Cell cytotoxicity of *male*, *Hdmpz*, *fum*, *3-AMpy* and $ZnCl_2$ in PBMC cells. Data represents % cell death as compared to respective untreated control.

Dose (μM)	% Cytotoxicity				
	male	*Hdmpz*	*fum*	*3-AMpy*	$ZnCl_2$
0.01	0	0	0	0	0
0.1	0	0	0	0	0
0.5	0	0	0	0	0
1	0	0	0	0	0
5	0	0	0	0	0
10	0	0	0	0	0
50	0	0	0	0	4
100	0	0	0	0	6
200	0	0	0	0	7

300	2	2	0	3	8
400	2	3	2	3	10
500	3	3	4	4	12
IC_{50}	**IC_{50}** could not be calculated due to very low cytotoxicity				

Table S4 Intermolecular interactions between receptors and compounds **1** and **2**. The reference ligands were used from PDB entry file of respective receptor.

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**	1	Arg104	-123
		Compound **2**	3	Arg104, Asp100, Leu94, Thr93	-143
2	BCL-XL (2YXJ)	Reference ligand	4	Gly138, Glu129	-145
		Compound **1**	3	Glu129, Arg139	-109
		Compound **2**	3	Glu129, Tyr101, Ala149	-134
3	MCL-1 (5VKC)	Reference ligand	4	Arg263, Leu267	-176
		Compound **1**	2	Arg262	-117
		Compound **2**	4	Arg262, Leu267, Arg263	-154

Supplementary references

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