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

Supplementary Information

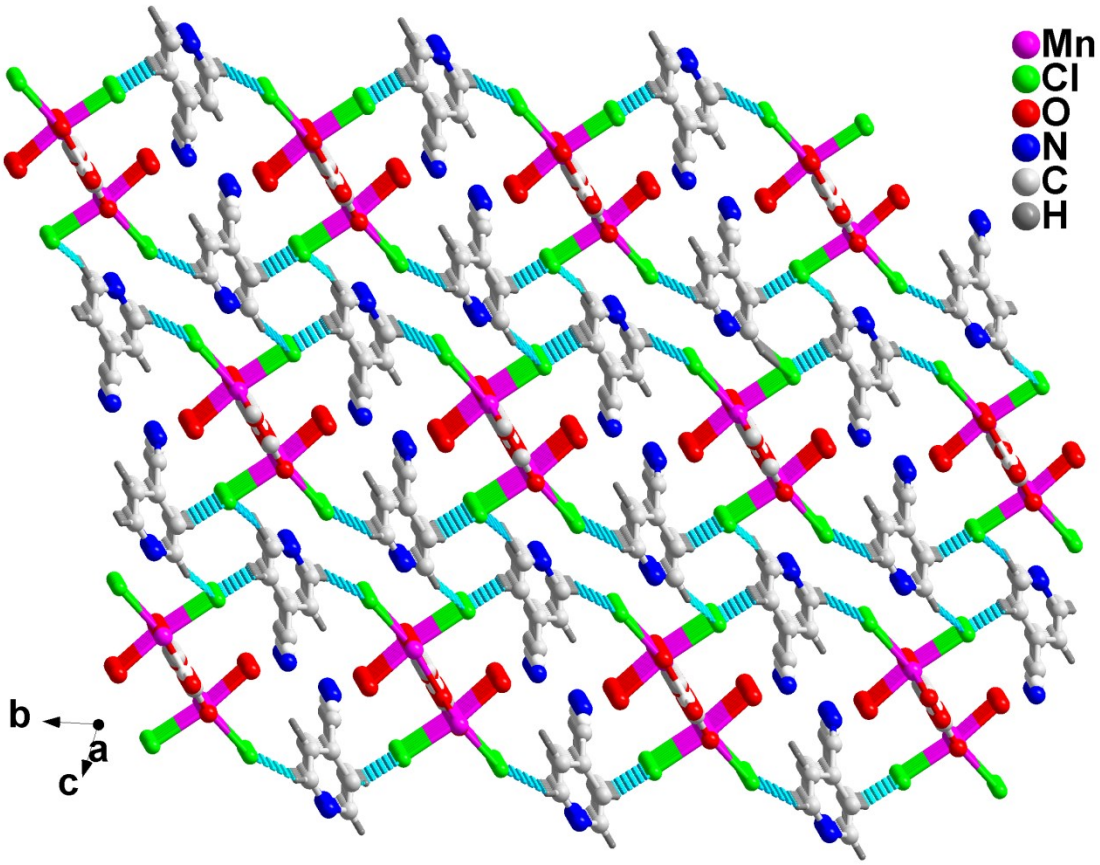


Fig. **S1** 3D network structure of the polymer **1** with channels along crystallographic *c* direction

Table S1 Selected parameters for weak hydrogen bonding interactions in complex **1**

D–H···A	H···A	D···A	D–H···A	Symmetry Code
O3–H3A···Cl2	2.27	3.162(7)	172	-x, -y, 2-z
C4–H4···N2	2.70	3.584(1)	154	2-x,-y,2-z
C7–H7A···Cl2	2.68	3.590(1)	159	x+1,+y,+z
C6–H6···Cl1	2.75	3.487(2)	133	-x+1,-y+1,-z+1

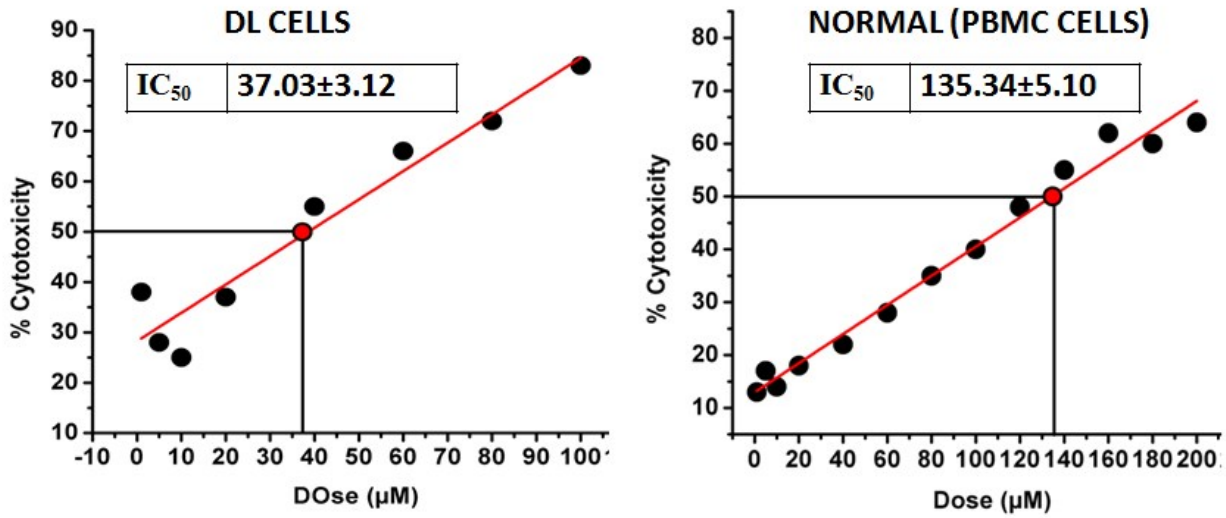


Fig. **S2** IC_{50} values of compound **1** in cancer (DL cells) and normal (PBMC) cells.

Table S2 Cell cytotoxicity of compound **1**, metal salt and 4-CNpy in DL cells. Data represents % cell death as compared to respective untreated control. ND: Not determined.

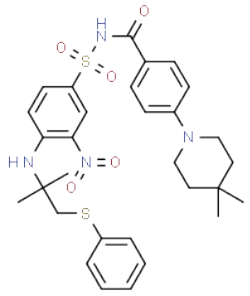
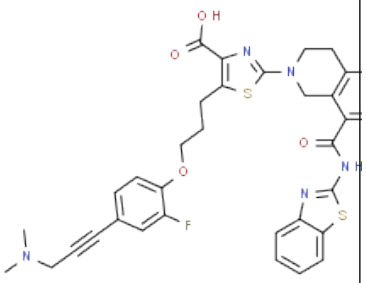
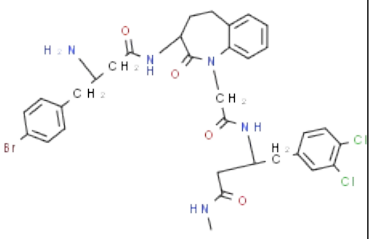
Dose (µM)	% Cytotoxicity		
	Compound **1**	Metal salt	4-CNpy
1	38	0	0
5	28	0	0
10	25	0	0
20	37	0	0
40	55	2	3
60	66	4	4
80	72	5	5
100	83	5	7
IC_{50}	**37.03±3.12**	ND	ND

Table S3 Cell cytotoxicity of compound **1**, metal salt and 4-CNpy in normal (PBMC) cells. Data represents % cell death as compared to respective untreated control. ND: Not determined.

Dose (µM)	% Cytotoxicity		
	Compound **1**	Metal salt	4-CNpy
1	13	0	0
5	17	0	0

10	14	0	0
20	18	0	0
40	22	2	3
60	28	2	4
80	35	4	4
100	40	5	5
120	48	5	5
140	55	5	4
160	62	6	6
180	70	6	6
200	78	6	7
IC_{50}	**135.34±5.11**	ND	ND

Table S4 The binding affinity demonstrated that compound **1** interacted with anti-apoptotic proteins with strong binding energy and the results were comparable with reference inhibitors.

Receptors	**Reference ligands**	**Structures of the reference ligands**	**Docking score of the reference ligands**	**Docking scores of compound 1**
BCL-2 (PDB ID: 2O22)	**N-[(4-{[1,1-dimethyl-2-(phenylthio)ethyl]amino}-3-nitrophenyl)sulfonyl]-4-(4,4-dimethylpiperidin-1-yl)benzamide**		-172	-148
BCL-XL (PDB ID: 4QVX)	**2-[8-(1,3-benzothiazol-2-ylcarbamoyl)-3,4-dihydroisoquinolin-2(1H)-yl]-5-(3-{4-[3-(dimethylamino)prop-1-yn-1-yl]-2-fluorophenoxy}propyl)-1,3-thiazole-4-carboxylic acid**		-145	-120
MCL-1 (PDB ID: 5KU9)	**(3~{S})-3-azanyl-4-(4-bromophenyl)-~{N}-[(3~{S})-1-[2-[[(2~{R})-1-(3,4-dichlorophenyl)-4-(methylamino)-4-oxidanylidene-butan-2-yl]amino]-2-oxidanylidene-ethyl]-2-oxidanylidene-4,5-dihydro-3~{H}-1-**		-132	-98

	benzazepin-3-yl]butanamide			