Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

For

Zinc (II) Complexes Containing Bis-benzimidazole Derivatives as a New Class of Apoptosis Inducers That Trigger DNA Damage-mediated P53 Phosphorylation in Cancer Cells

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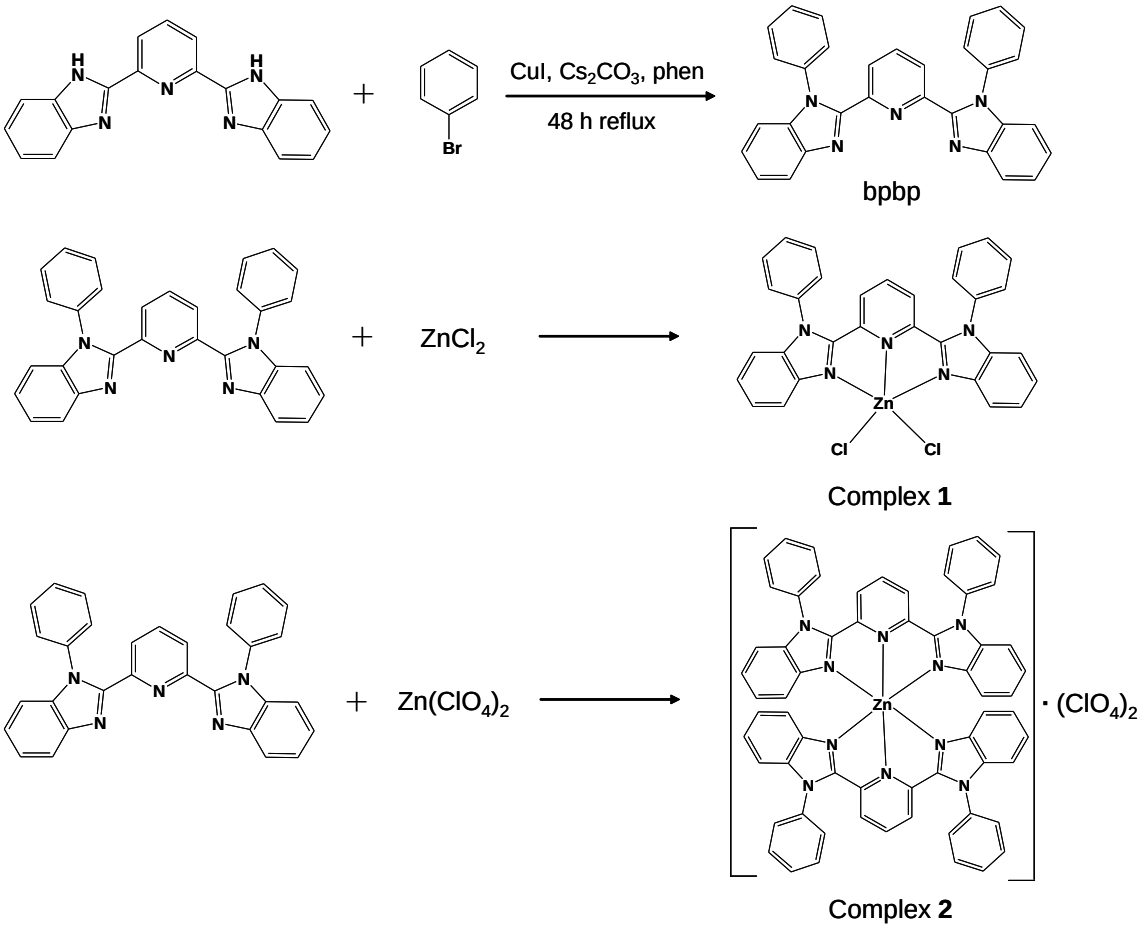
EXPERIMENTAL SECTION

Synthesis and characterizations

The Schematic routes for the synthesis of ligand and complexes were shown in **Scheme S1**.



Scheme S1. Schematic routes for synthesis of ligand (bpbp), complex **1** and **2**.

RESULTS

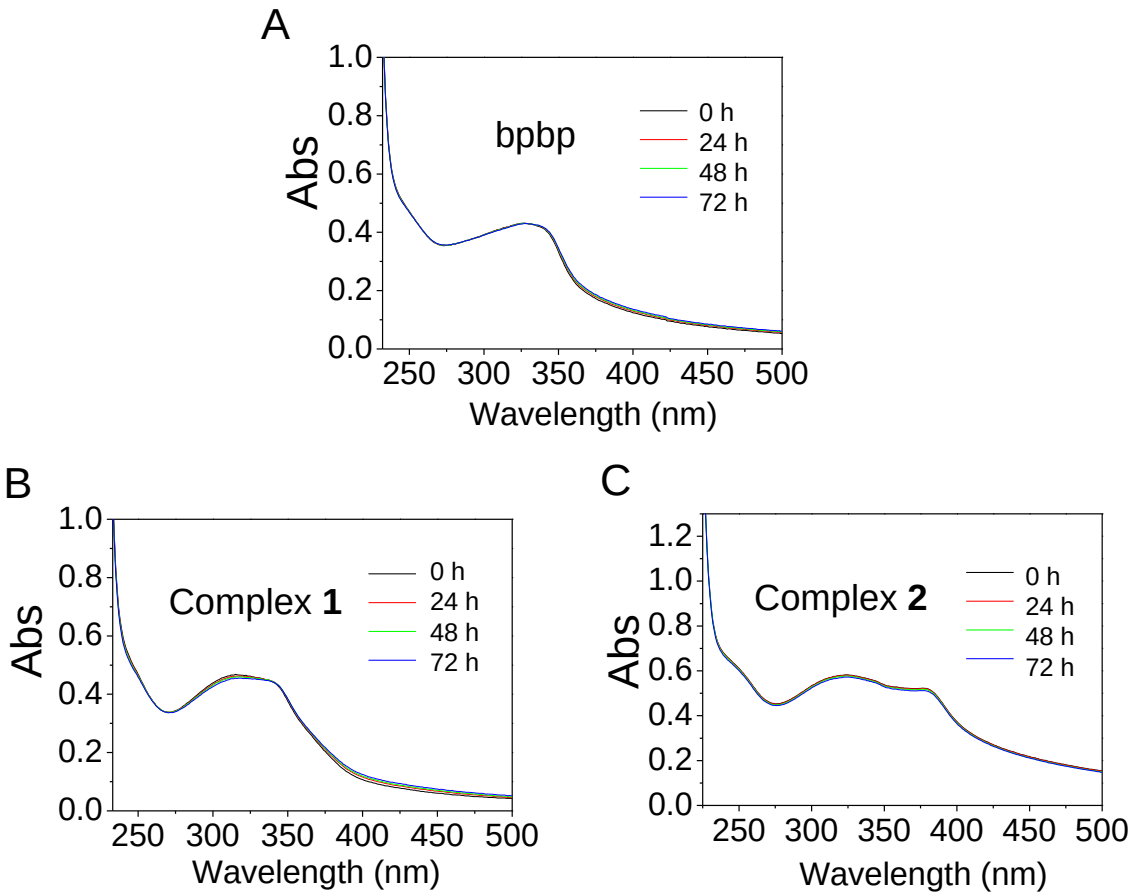


Figure S1. UV-Vis absorption spectra of ligand and complexes in DMSO during incubation at 25 °C.

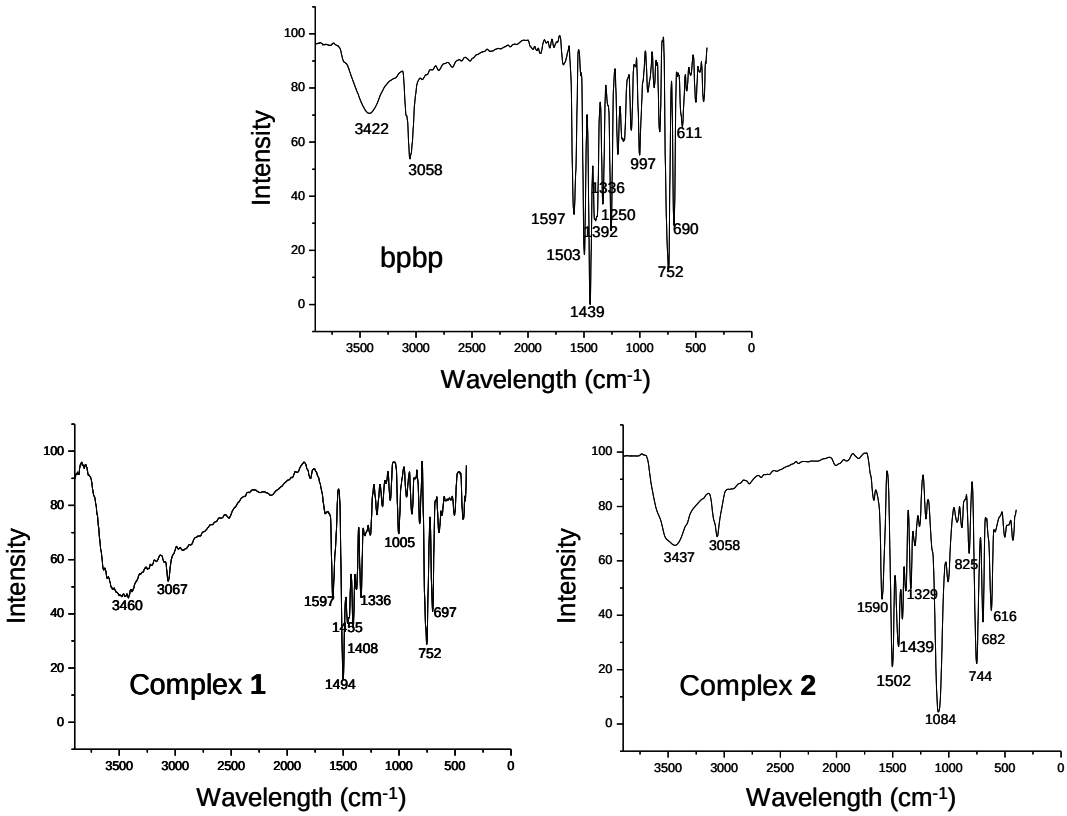


Figure S2. The IR spectra of ligand and complexes.

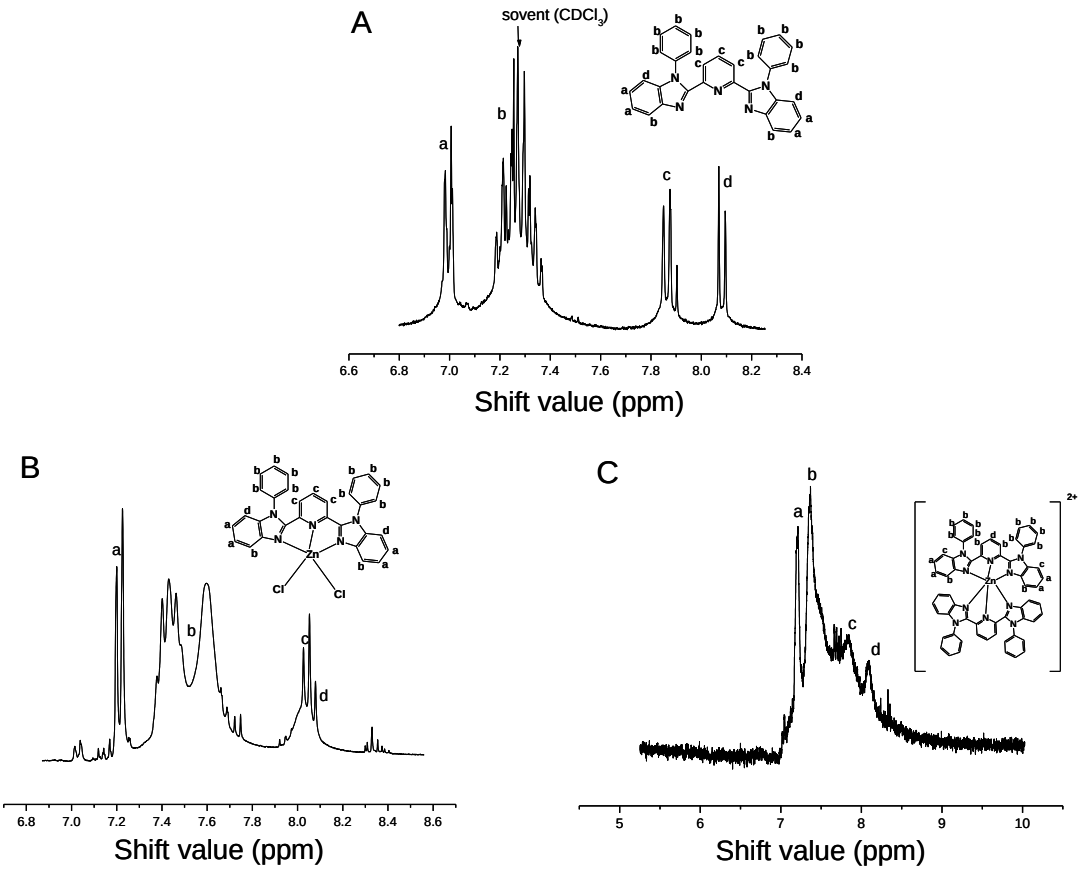


Figure S3. The 'HNMR spectra of bpbp (A), complex **1** (B) and **2** (C).

Table S1. Selected crystallographic data for bpbp, complex **1** and complex **2**

	bpbp	Complex **1**	Complex **2**
Formula	$C_{31}H_{21}N_5$	$C_{31}H_{21}C_{l2}N_5Zn$	$C_{64}H_{50}Cl_2N_{10}O_{10}$
formula weight	463.53	599.80	1255.41
Crystal system	Orthorhombic	Monoclinic	Triclinic
space group	Pbcn	Cc	P-1
a / Å	10.9303(12)	15.743(2)	11.1528(10)
b / Å	11.0153(12)	9.4359(14)	13.9924(12)
c / Å	19.836(2)	17.663(3)	19.1852(17)
α / °	90	90	82.0960(10)
β / °	90	90.993(2)	76.3430(10)
γ / °	90	90	89.2320(10)
V / $Å^3$	2388.3(4)	2623.3(7)	2881.1(4)
Z	4	4	2
Density calc.$Mg.m^{-3}$	1.289	1.519	1.447
Absorption coefficient (mm^{-1})	0.078	1.172	0.590
F(000)	968	1224	1296
Crystal size	0.45, 0.41, 0.23	0.44, 0.34, 0.13	0.36, 0.25, 0.18
Theta range for data collection	2.05 to 27.05	2.31 to 27.02	1.10 to 27.11
Limiting indices	-13<=h<=13 -7<=k<=14 -25<=l<=23	-20<=h<=12 -12<=k<=11 -21<=l<=22	-14<=h<=14 -17<=k<=17 -24<=l<=24
Reflections collected / unique	13313 / 2618 [R(int) = 0.0234]	7229/3936 [R(int) = 0.0233]	24439/12375 [R(int)= 0.0283]
Data / restraints / parameters	2618 / 0 / 164	3936 / 2 / 353	12375 / 22 / 811
GOF on F^2	1.032	1.095	1.056
Max. and min. transmission	0.9822 , 0.9656	0.8626 , 0.6267	0.838, 0.899
Final R indices[I>2sigma(I)]	R1 = 0.0352, wR2= 0.0830	R1= 0.0287, wR2 = 0.0631	R1 = 0.0680, wR2 = 0.1772
R indices (all, data) R_1, wR_2	R1 = 0.0498, wR2 = 0.0929	R1= 0.0351, wR2= 0.0663	R1 = 0.0759 wR2 =0.2068
Largest diff. peak and hole $e.Å^{-3}$	0.215 ,-0.204	0.275,-0.293	1.928, -1.974

Table S2. Selected bond lengths (Å) and angles (°) for bpbp

Bend lengths		**Bend angles**	
N(1)-C(3)$^{\#1}$	1.3393(14)	N(1)	1.3393(14)
C(4)-N(3)	1.3144(15)	C(4)	1.3794(15)
N(3)-C(5)	1.3890(16)	C(10)	1.3857(14)
N(2)-C(11)	1.4364(15)	--	--
N(3)-C(4)-N(2)	113.67(10)	N(2)	105.30(10)
N(2)-C(4)-C(3)	121.72(10)	C(4)	106.05(9)
C(4)-N(2)-C(11)	127.19(10)	C(10)	126.67(10)
C(12)-C(11)-N(2)	119.51(11)	C(16)	119.33(11)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, y, -z+1/2

Table S3. Selected bond lengths (Å) and angles (°) for complex **1**

Bend lengths		**Bend angles**	
Zn(1)-N(4)	2.133(3)	Zn(1)-N(1)	2.139(3)
Zn(1)-N(3)	2.237(3)	Zn(1)-Cl(1)	2.2558(10)
Zn(1)-Cl(2)	2.2731(10)	--	--
N(4)-Zn(1)-N(1)	144.52(10)	N(1)-Zn(1)-N(3)	72.10(9)
N(4)-Zn(1)-N(3)	72.44(9)	N(4)-Zn(1)-Cl(1)	97.27(8)
N(1)-Zn(1)-Cl(1)	98.35(8)	N(3)-Zn(1)-Cl(1)	118.73(8)
N(4)-Zn(1)-Cl(2)	100.17(8)	N(1)-Zn(1)-Cl(2)	99.98(8)
N(3)-Zn(1)-Cl(2)	122.79(8)	Cl(1)-Zn(1)-Cl(2)	118.48(4)

Table S4. Selected bond lengths (Å) and angles (°) for complex **2**

Bend lengths		**Bend angles**	
Zn(1)-N(3)	2.117(3)	Zn(1)-N(6)	2.140(3)
Zn(1)-N(8)	2.142(3)	Zn(1)-N(1)	2.143(3)
Zn(1)-N(4)	2.168(3)	Zn(1)-N(9)	2.191(3)
N(3)-Zn(1)-N(6)	111.78(12)	--	--
N(6)-Zn(1)-N(8)	75.23(12)	N(3)-Zn(1)-N(1)	76.01(12)
N(6)-Zn(1)-N(1)	89.60(12)	N(8)-Zn(1)-N(1)	109.81(12)
N(3)-Zn(1)-N(4)	75.46(12)	N(3)-Zn(1)-N(8)	171.33(12)
N(8)-Zn(1)-N(4)	98.32(12)	N(6)-Zn(1)-N(4)	102.75(12)
N(3)-Zn(1)-N(9)	98.79(12)	N(1)-Zn(1)-N(4)	151.41(13)
N(8)-Zn(1)-N(9)	74.69(12)	N(6)-Zn(1)-N(9)	149.21(13)
N(4)-Zn(1)-N(9)	87.99(12)	N(1)-Zn(1)-N(9)	94.42(12)